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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
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NEWS 3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 5	JAN 28	MARPAT searching enhanced
NEWS 6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS 7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
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NEWS 11	FEB 25	IFIREF reloaded with enhancements
NEWS 12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS 13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS 14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS 15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS 16	MAR 31	CA/CAplus and CASREACT patent number format for U.S. applications updated
NEWS 17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS 18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS 20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS 21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS 22	APR 28	IMSRESEARCH reloaded with enhancements
NEWS 23	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS 24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS 25	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS 26	JUN 06	KOREAPAT updated with 41,000 documents

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 15:00:57 ON 11 JUN 2008

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:01:10 ON 11 JUN 2008
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 JUN 2008 HIGHEST RN 1026855-74-2
DICTIONARY FILE UPDATES: 9 JUN 2008 HIGHEST RN 1026855-74-2

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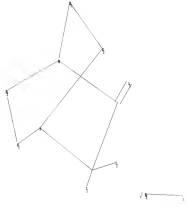
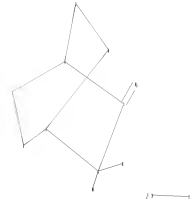
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10590054.str





chain nodes :
10 12 13 17 18
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
5-10 6-17 6-18 12-13
ring bonds :
1-2 1-6 1-8 2-3 3-4 4-5 4-7 5-6 7-8
exact/norm bonds :
1-2 1-6 1-8 2-3 3-4 4-5 4-7 5-6 5-10 6-17 6-18 7-8 12-13

G1:O,S,N

G2:H,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 12:CLASS
13:CLASS 17:CLASS 18:CLASS

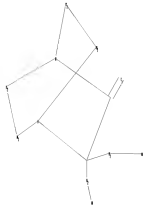
L1   STRUCTURE UPLOADED

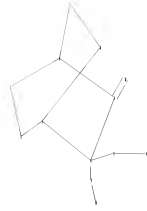
=> d l1
L1 HAS NO ANSWERS
L1   STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Program Files\Stnexp\Queries\10590054b.str





```
chain nodes :
10  13  14  15  16
ring nodes :
1  2  3  4  5  6  7  8
chain bonds :
5-10  6-13  6-15  13-14  15-16
ring bonds :
1-2  1-6  1-8  2-3  3-4  4-5  4-7  5-6  7-8
exact/norm bonds :
1-2  1-6  1-8  2-3  3-4  4-5  4-7  5-6  5-10  7-8
exact bonds :
6-13  6-15  13-14  15-16
```

G1:O,S,N

G2:H

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 13:CLASS
14:CLASS 15:CLASS 16:CLASS

L2 STRUCTURE UPLOADED

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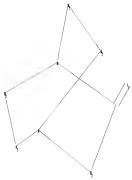
Uploading C:\Program Files\Stnexp\Queries\10590054c.str



```
chain nodes :
10
ring nodes :
1  2  3  4  5  6  7  8
chain bonds :
5-10
ring bonds :
1-2  1-6  1-8  2-3  3-4  4-5  4-7  5-6  7-8
exact/norm bonds :
5-10
exact bonds :
1-2  1-6  1-8  2-3  3-4  4-5  4-7  5-6  7-8
```

```
isolated ring systems :
containing 1 :


G1:O,S,N

G2:H

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  10:CLASS



L3      STRUCTURE UPLOADED

=> s l1 full
FULL SEARCH INITIATED 15:02:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    84668 TO ITERATE

100.0% PROCESSED    84668 ITERATIONS                                925 ANSWERS
SEARCH TIME: 00.00.01

L4          925 SEA SSS FUL L1

=> s l2 full
FULL SEARCH INITIATED 15:03:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       49 TO ITERATE

100.0% PROCESSED       49 ITERATIONS                                  2 ANSWERS
SEARCH TIME: 00.00.01

L5            2 SEA SSS FUL L2

=> s l3 full
FULL SEARCH INITIATED 15:03:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    46039 TO ITERATE

100.0% PROCESSED    46039 ITERATIONS                                436 ANSWERS
SEARCH TIME: 00.00.01

L6          436 SEA SSS FUL L3

=> s l4 not l5 full
L7         923 L4 NOT L5

=> s l7 not l6 full
L8         487 L7 NOT L6

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                ENTRY    SESSION
FULL ESTIMATED COST                            536.00     536.21

FILE 'CAPLUS' ENTERED AT 15:04:27 ON 11 JUN 2008
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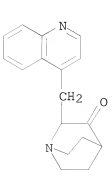
FILE COVERS 1907 - 11 Jun 2008 VOL 148 ISS 24
FILE LAST UPDATED: 10 Jun 2008 (20080610/ED)

=> s l8 full
L9 160 L8

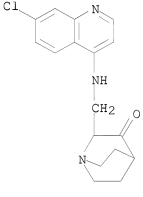
=> d ibib abs hitstr 160

L9 ANSWER 160 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1940:708 CAPLUS
DOCUMENT NUMBER: 34:708
ORIGINAL REFERENCE NO.: 34:110b-g
TITLE: Synthesis of 5-substituted rubans
AUTHOR(S): Clemo, G. R.; Hoggarth, E.
SOURCE: Journal of the Chemical Society (1939) 1241-4
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 34:708
GI For diagram(s), see printed CA Issue.
AB Lepidine (40 g.), 44 g. chloral and 100 cc. C5H5N, warmed at 85-90° for 2 hrs., give 80% of γ-trichloro-β-hydroxy-α-(4-quinolyl)propane, m. 178°; adding 65 g. during 2 hrs. to 65 g. KOH in 300 cc. absolute EtOH on the water bath gives 80% of β-4-quinolylacrylic acid, m. 270°; oxidation of 36 g. acid in a solution of 14 g. Na2CO3 in 500 cc. H2O with 60 g. KMnO4 in 1.5 l. H2O at -10° gives 58% (overall yield 38-40%) of quinoline-4-aldehyde (I), b4 122-3°, m. 52°; picrate, yellow, m. 179° (contains 1 mole of EtOH). 3-Ketoquinuclidine (II) (C. and Metcalfe, C. A. 32, 1701.3, term it the 2-derivative) and BzH in absolute EtOH containing piperidine or KOH, refluxed 8-10 hrs., give 2-benzylidene-3-ketoquinuclidine, light yellow, m. 133°; phenylhydrazone, light yellow, m. 184°. II (0.5 g.) and 0.8 g. I in AcOH, saturated with dry HCl at 0°, and after 2-3 hrs. warmed at 80-5° for 8 hrs., give 0.2 g. 5-keto-6,9-rubanene (III), deep yellow, m. 153°; III results in 0.4-0.5 g. yield from 0.5 g. II and 0.65 g. I with piperidine acetate in absolute EtOH; after keeping 60 hrs. in the cold and then heating momentarily to boiling; picrate, red, m. 209°; chloroplatinate, orange needles, decompose above 260° without melting. Catalytic reduction of 0.5 g. of III with Pd-C in MeOH gives 0.3 g. of 5-ketoruban (IV (R = 4-quinolyl)), m. 125-6°; phenylhydrazone, yellow, m. 198°; picrate, deep yellow, m. 168°. Reduction of 0.5 g. of IV with (iso-PrO)3Al in iso-PrOH gives 0.3 g. of ruban-5-ol, m. 198°; picrate, yellow, m. 188-9°. IV (0.3 g.) with EtMgI in Et2O at -10° gives 0.03-0.05 g. of 5-ethylruban-5-ol (V), m. 139°; picrate, yellow, m. 161°. III (0.8 g.) and EtMgI in Et2O at 0° give 0.05 g. of a compound C19H22ON2, m. 164°; picrate, deep yellow, m. 150°; crystalline compds. could not be prepared with N2H4.H2O, PhNHNH2, NH2OH or H2NNHCONH2; no Me2CO was detected in an attempted reduction with (iso-PrO)3Al and the compound was unchanged on boiling with HCO2H or Ac2O; catalytic reduction did not yield V.
IT 24177-70-6, 3-Quinuclidinone, 2-(4-quinolylmethyl)-
(and derivs.)
RN 24177-70-6 CAPLUS
CN 11-Norcinchonan-7-one, (8ξ)- (9CI) (CA INDEX NAME)

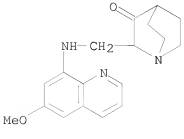


```
=> d ibib abs hitstr 150-159
```

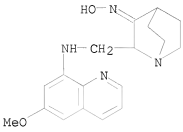
L9 ANSWER 150 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:430341 CAPLUS
DOCUMENT NUMBER: 71:30341
ORIGINAL REFERENCE NO.: 71:5589a,5592a
TITLE: Antimalarials. Some quinuclidine derivatives of 7-chloro-4-aminoquinoline and 6-methoxy-8-aminoquinoline
AUTHOR(S): Singh, Tara; Stein, Robert G.; Koelling, Harlan H.; Hoops, John F.; Biel, John H.
CORPORATE SOURCE: Res. Lab., Aldrich Chem. Co., Inc., Milwaukee, WI, USA
SOURCE: Journal of Medicinal Chemistry (1969), 12, 524-6
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Thirteen quinoline compds. containing quinuclidine rings in side chains were prepared and tested for their antimalarial activity against Plasmodium berghei in mice. 7-Chloro-4-(3-oxoquinuclidinyl-2-methyleneamino)quinoline (I) and 7-chloro-4-(3-hydroxyquinuclidinyl-2-methyleneamino)quinoline (II) were curative; I cured 2 mice at 160 mg./kg. and all 5 in the test at 640 mg./kg., while II showed slight activity at 160 and 320 mg./kg. and cured all 5 mice at 640 mg./kg. All other compds. were inactive and toxic.
IT 21566-68-7P 22776-50-7P 22776-52-9P
22950-03-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21566-68-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(7-chloro-4-quinolinyl)amino]methyl]- (CA INDEX NAME)



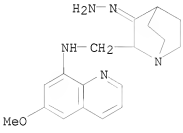
RN 22776-50-7 CAPLUS
CN 3-Quinuclidinone, 2-[[(6-methoxy-8-quinolyl)amino]methyl]- (8CI) (CA INDEX NAME)



RN 22776-52-9 CAPLUS
CN 3-Quinuclidinone, 2-[[(6-methoxy-8-quinolyl)amino]methyl]-, oxime (8CI) (CA INDEX NAME)



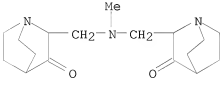
RN 22950-03-4 CAPLUS
CN 3-Quinuclidinone, 2-[[(6-methoxy-8-quinolyl)amino]methyl]-, hydrazone (8CI) (CA INDEX NAME)



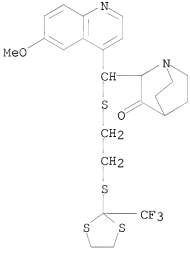
L9 ANSWER 151 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:459119 CAPLUS
DOCUMENT NUMBER: 69:59119
ORIGINAL REFERENCE NO.: 69:11047a,11050a
TITLE: 2-Methylene-3-quinuclidinone
INVENTOR(S): Biel, John H.; Hopps, Harvey B.; Bader, Henryk
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 2 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3384641	A	19680521	US 1967-668941	19670919
PRIORITY APPLN. INFO.:			US 1967-668941 A	19670919

GI For diagram(s), see printed CA Issue.
AB The title compound (I) is prepared by heating the Mannich reaction product of 3-quinuclidinone (II), Me2NH, and HCHO; it is used to sep. tertiary from primary and secondary amines. Thus, 200 g. II, 270 g. 40% Me2NH, 194.8 g. 37% HCHO, 250 ml. EtOH, and 100 ml. water was refluxed 1 hr., held 17 hrs. at 70°, and worked up to give 203 g. I, b7 91-2°, n2D0 1.5110; HCl salt m. 284-8°. A mixture of pyridine and piperidine was separated by distillation in the presence of I. The piperidine distilled only after its reaction product with I decomposed MeNH2 was also purified by adding 13.7 g. I in 20 ml. MeOH to 3.88 g. 40% aqueous MeNH2 and heating 1 hr. at 50° to give 11 g. 2,α'-methyliminobis(2-methyl-3-quinuclidinone) monohydrate, m. 90-2°, which was decomposed by gentle heating to pure MeNH2, leaving I as a residue.
IT 19576-25-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19576-25-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2'-[(methylimino)bis(methylene)]bis- (9CI) (CA INDEX NAME)



L9 ANSWER 152 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:427579 CAPLUS
DOCUMENT NUMBER: 69:27579
ORIGINAL REFERENCE NO.: 69:5155a,5158a
TITLE: Synthetic quinine analogs. I. Synthesis and some chemical transformations of 6'-methoxy-7-oxo-8-rubene
AUTHOR(S): Bender, D. R.; Coffen, D. L.
CORPORATE SOURCE: Univ. of Colorado, Boulder, CO, USA
SOURCE: Journal of Organic Chemistry (1968), 33(6), 2504-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB NaOEt-catalyzed condensation of 6-methoxyquinoline-4-carboxaldehyde with 3-quinuclidinone produces 6'-methoxy-7-oxo-8-rubene (I) in high yield. Of the 2 possible geometrical isomers, only that with the ketone function trans to the quinoline ring is formed. Reduction of I affords an allylic alc. whose p-nitrobenzoate is completely isomerized to the opposite geometrical isomer in refluxing HOAc. I is not ketalized by 1,2-ethanedithiol in refluxing F3CCO2H involving 1 mol. of ketone, 2 of 1,2-ethanedithiol, and 1 of F3CCO2H. A by-product of the reaction results from the condensation of 3 mols. of 1,2-ethanedithiol with 2 of F3CCO2H. Pyrazoline derivs. of I resulting from 1,3-dipolar addition of CH2N2 and condensation with hydrazine are described. 24 references.
IT 16526-37-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16526-37-7 CAPLUS
CN Orthoacetic acid, trifluorotrithio-, cyclic ethylene ester, ester with 2-[[(2-mercaptoethyl)thio](6-methoxy-4-quinolyl)methyl]-3-quinuclidinone, (±)- (8CI) (CA INDEX NAME)

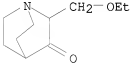


L9 ANSWER 153 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:84473 CAPLUS
DOCUMENT NUMBER: 64:84473
ORIGINAL REFERENCE NO.: 64:15837a-b
TITLE: Systems with bridgehead nitrogen. β-Ketols of the 1-azabicyclo[2.2.2]octane series
AUTHOR(S): Nielsen, Arnold T.
CORPORATE SOURCE: Chem. Div., U.S. Naval Ordnance Test Sta., China Lake, CA
SOURCE: Journal of Organic Chemistry (1966), 31(4), 1053-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

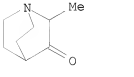
AB The prepns. and chemical behavior of the β-ketols incorporating the 1-azabicyclo [2.2.2] octane ring are described. Three different structural types are represented in this study. Methylolation of 3-quinuclidinone with excess formaldehyde (potassium carbonate catalyst under appropriate conditions) led to 2,2-bismethylol-3-quinuclidinone (I) or 2-methylene-3-quinuclidinone (II). 2-Methylol-3-quinuclidinone (III) was prepared by hydration of II cation. Starting with 4-acetylpiperidine and its N-benzyl derivative, syntheses of 4-hydroxymethyl-3-quinuclidinone (IV) and 4-acetyl-3-quinuclidinol (V) were achieved. The bridgehead IV was extremely stable whereas V underwent facile retrograde aldolization in basic media. I readily loses one methylol group in base leading to III, which dehydrates with extreme ease rather than undergo demethylolation.

IT 5291-13-4P, 3-Quinuclidinone, 2-(ethoxymethyl)- 5291-14-5P
, 3-Quinuclidinone, 2-methyl- 5291-27-0P, 3-Quinuclidinone,
2-(hydroxymethyl)- 5291-32-7P, 3-Quinuclidinone,
2-(hydroxymethyl)-2-(methoxymethyl)- 5291-33-8P,
3-Quinuclidinone, 2-(ethoxymethyl)-, picrate 5291-34-9P,
3-Quinuclidinone, 2-methyl-, picrate 5291-35-0P,
3-Quinuclidinone, 2-(hydroxymethyl)-, hydrochloride
RL: PREP (Preparation)
(preparation of)

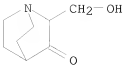
RN 5291-13-4 CAPLUS
CN 3-Quinuclidinone, 2-(ethoxymethyl)- (7CI, 8CI) (CA INDEX NAME)



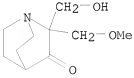
RN 5291-14-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-methyl- (CA INDEX NAME)



RN 5291-27-0 CAPLUS
CN 3-Quinuclidinone, 2-(hydroxymethyl)- (7CI, 8CI) (CA INDEX NAME)



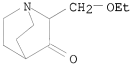
RN 5291-32-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)- (CA INDEX NAME)



RN 5291-33-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(ethoxymethyl)-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

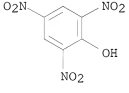
CM 1

CRN 5291-13-4
CMF C10 H17 N O2



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



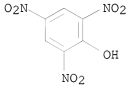
RN 5291-34-9 CAPLUS
CN 3-Quinuclidinone, 2-methyl-, picrate (7CI, 8CI) (CA INDEX NAME)

CM 1

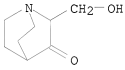
CRN 5291-14-5
CMF C8 H13 N O

CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



RN 5291-35-0 CAPLUS
CN 3-Quinuclidinone, 2-(hydroxymethyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



● HCl

L9 ANSWER 154 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:9663 CAPLUS
DOCUMENT NUMBER: 60:9663
ORIGINAL REFERENCE NO.: 60:1697e-h,1698a-h,1699a
TITLE: Quinuclidine series. VII. Solvolysis of 2-(α-chlorobenzyl)quinuclidine. The heterocinchonine rearrangement
AUTHOR(S): Braschler, V.; Grob, C. A.; Kaiser, A.
CORPORATE SOURCE: Univ. Basel, Switz.
SOURCE: Helvetica Chimica Acta (1963), 46(7), 2646-58
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 60:9663

AB cf. CA 53, 4278e. The rate and the products of the hydrolysis of 2-(α-chlorobenzyl)quinuclidine (I) do not provide evidence for the participation of the quinuclidine N in the ionization step, and no product derived from a heterocinchonine rearrangement could be isolated. 2-Benzyl-2-dehydroquinuclidine (II) and 2-benzylidenequinuclidine (III) possess abnormal spectral and chemical properties ascribable to steric inhibition of the vinylamine-type mesomerism. Et isonicotinate (151 g.) and 167 g. BrCH2CO2Et in 500 cc. EtOH kept at room temperature overnight, refluxed 4 hrs., hydrogenated 0.5-1 hr. at 90°/100 atmospheric over 15 g. 10% Pd-C, filtered, the filtrate evaporated at 50-60°, the semicryst. residue treated with cooling and shaking with 500 cc. cold H2O, 500 cc. CHCl3, and 150 g. K2CO3 in 250 cc. H2O, and the organic layer worked up yielded 180-90° 4-carbethoxy-1-carbethoxymethylpiperidine (IV), b0.2 111-13°, n20D 1.4585, d1515 1.057. IV (100 g.) in 250 cc. absolute MePh added dropwise during 1.5 hrs. to KOEt (from 39.096 g. K and 60 cc. EtOH in 162 cc. dry MePh) the mixture stirred 4 hrs. at 130°, cooled, the MePh decanted, extracted with 50 cc. H2O, the residue dissolved in 300 cc. EtOH, combined with the aqueous extract, the solution adjusted with 10N HCl with cooling and stirring to pH 7 below 30°, cooled to 0°, filtered, the filtrate adjusted with about 2 cc. AcOH to pH 4, concentrated to about 200 cc., treated with 20 cc. saturated aqueous KHCO3, and extracted with CHCl3 yielded 57 g. 2-carbethoxy-3-quinuclidone (V), b0.02 98-103°, m. 116-20° (absolute EtOH-Et2O). V (20 g.), 80 cc. dry Et3N, and 100 cc. absolute EtOH hydrogenated over about 5 g. Raney Ni under ambient conditions yielded 10.9 g. 2-carbethoxy-3-hydroxyquinuclidine (VI) isomer A (VII), m. 147-8° (Me2CO), (sublimation); the filtrate was evaporated and the cryst, residue (9 g.) chromatographed on 200 g. Al2O3 to give 2.34 g. VII, 4.7 g. isomer mixture, m. 72-105°, and 1.98 g. VI isomer B, m. 100-2°; VI.MeI, m. 175-8° (decomposition) (EtOH-Et2O). VI (21.1 g.) and 150 cc. Ac2O refluxed 6 hrs., the mixture evaporated, the oily residue partitioned between 200 cc. Et2O and 50 cc. 2N HCl, the Et2O phase extracted with 2N HCl, the combined aqueous solns. saturated with solid K2CO3, and extracted with Et2O gave 14.4 g. 2-carbethoxy-2-dehydroquinuclidine (VIII), b12 128-30°, n25D 1.4955, and 1.1 g. acetate of VI, b12 130-63°. VIII (12.7 g.) in 65 cc. EtOH hydrogenated 1 hr. over 600 mg. 10% Pd-C under ambient conditions yielded 12.1 g. 2-carbethoxyquinuclidine, b11 119-20°, n25D 1.4752, b11 119-20°; picrate m. 120° (EtOH). VIII (10 g.) and 150 cc. saturated NH3-MeOH heated 15 hrs. at 100° in an autocalve gave 7.5 g. 2-CONH2 analog (IX) of VIII, m. 178-81° (Me2CO). IX (5.45 g.) in 50 cc. MeOH and 25 cc. H2O hydrogenated 2 hrs. over Raney Ni W-7 under ambient conditions yielded 4.9 g. 2-carbamoylquinuclidine (X), m. 148-9°(Me2CO). 2-Carbethoxyquinuclidine (1.2 g.) and 10 cc. NH3-MeOH (saturated at 20°) heated 48 hrs. at 100° in a sealed tube gave 0.81 g. X, m. 145-6° (Me2CO). IX (5.6 g.) in 45 cc. Et3N

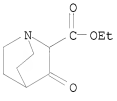
and 25 cc. CHCl3 mixed with 10.5 g. P2O5 g. and 50 g. sand, refluxed 30 hrs., cooled, the supernate decanted, the residual oil washed with Et2O, the residue treated with saturated aqueous K2CO3 and extracted with Et2O, and the combined washings, and decantate worked up yielded 0.92 g. unreacted IX, m. 177-80°; the mother liquor distilled gave 2 g. 2-CN analog of VIII, b11 120-3°, n 24.5D 1.5068. X (12.2 g.), 22.5 g. P2O5, and 50 g. sand refluxed 26 hrs. with 90 cc. dry Et3N and 60 cc. dry CHCl3 and similarly worked up yielded 8.25 g. 2-cyanoquinuclidine (XI), b13 105-21°; picrate m. 216-26° (decomposition) (Me2CO-EtOH); XI.MeI m. 247-50° (decomposition) (absolute EtOH). X (9.4 g.), 50 cc. Ac2O, and 50 cc. Et3N refluxed 10 hrs. yielded 4 g. XI, b13 105-21°. XI (17.4 g.) in 300 cc. dry C6H6 added dropwise during 1 hr. to PhMgBr from 6.5 g. Mg, 40.2 g. PhBr, and 170 cc. dry Et2O and the mixture refluxed 4 hrs. yielded 20.9 g. 2-benzoylquinuclidine (XII), m. 88-9.5° (Et2O); the residue from the mother liquor sublimed at 120-40°/11 mm. gave 1.35 g. XII, m. 86-9°; picrate m. 174-8° (EtOH); methiodide m. 196-8° (Me2CO). XII (1 g.) and 0.335 g. NH2OH.HCl in 20 cc. MeOH refluxed 24 hrs. yielded the oxime of XII, m. 194-5.5° with sublimation (AcOEt); picrate m. 194-8° with sublimation (EtOH) XII (4.0 g.) in 50 cc. dry Et2O added dropwise during 10 min. with stirring to 0.5 g. LiAlH4 in 50 cc. dry Et2O, the mixture refluxed 3 hrs., stirred 12 hrs. at room temperature, and decomposed with 30 cc. iced H2O and 25 cc. concentrated HCl yielded the mixed isomeric 2-(α-hydroxybenzyl)quinuclidine (XIII), which-recrystd. repeatedly from Me2CO gave 800 mg. isomer A (XIIIa), m. 142-4° [picrate m. 191-4° (EtOH)]; the residue (2.9 g.) from the mother liquor chromatographed on 60 g. Al2O3 gave the isomer B (XIIIb), m. 75-6.5° (petr. ether) [picrate m. 183-6° (EtOH)]. XIII (3 g.) and 30 cc. SOCl2 refluxed 12 hrs., the mixture evaporated, and the residue evaporated twice with C6H6 and fractionally recrystd. from absolute EtOH yielded I.HCl isomer A (Ia.HCl), m. 238-40° (absolute EtOH-Et2O) [picrate m. 183-6° (EtOH)], and I.HCl isomer B (Ib.HCl), m. 245-9.5° (decomposition) [picrate m. 173-4° (EtOH)]. Ia (1.89 g.) in 5 cc. absolute EtOH refluxed 3 hrs. with 3.5 g. KOH in 20 cc. absolute EtOH yielded 1.39 g. III isomer A (IIIa), b12 168-70° [picrate m. 149-50° and then 167-9° (EtOH)]. Ib (500 mg.) and 1 g. KOH in 10 cc. absolute EtOH refluxed 14 hrs. yielded 394 mg. oily III isomer B (IIIb) [picrate m. 162-3° and then 180-1° (iso-PrOH-Me2CO)]. Quinuclidone-HCl (8.5 g.) and 15 g. BzH refluxed 10 hrs. with 7.5 g. KOH in 150 cc. absolute EtOH yielded 8.07 g. 2-benzylidene-3-quinuclidone (XIV), m. 134-7° (MeOH) [picrate m. 180-4° (EtOH)]. XIV (11.05 g.) in 300 cc. MeOH hydrogenated under ambient conditions over Raney Ni, and the product fractionally recrystd. from Me2COMeOH yielded 7.7 g. 2-benzyl-3-hydroxyquinuclidine isomer A (XVa), m. 157-8° [picrate m. 128-32° (iso-PrOH); HCl salt m. 203-7° (MeOH-Me2CO-Et2O)]; the residue (2.85 g.) from the mother liquor chromatographed on 60 g. Al2O3 yielded 1.5 g. XV isomer B (XVb), m. 129-33° (Me2CO) [picrate, m. 159-62° (iso-PrOH)], and 1.3 g. mixed XVa and XVb. XVa (5 g.) and 50 cc. SOCl2 refluxed 70 hrs. gave 2 g. II, b0.005 62°, n23D 1.5485, which solidified at -15° [picrate m. 200-5° (Me2CO)], and 1.9 g. 2-benzyl-3-chloroquinuclidine, b0.005 73-5°, picrate m. 184-7° with a change to plates and then m. 201-3° (iso-PrOH). I.HCl (500 mg.) in 25 cc. EtOH hydrogenated about 2 hrs. over 50 mg. 10% Pd-C yielded 2-benzylquinuclidine-HCl (XVI.HCl), m. 268-9° (EtOH-Et2O) (with sublimation); picrate m. 184-6° (EtOH). IIIa or IIIb (200 mg.) in EtOH hydrogenated over Pd-C yielded XVI isolated as picrate, m. 183-6° (EtOH); XVI.HCl m. 270-2° (EtOH-Et2O). II (260 mg.) in 5 cc. EtOH hydrogenated over Raney Ni yielded XVI isolated as the picrate, m. 180.5-3.5° (iso-PrOH). I.HCl (2.0017 g.), 8 cc. N NaOH, 32.4 cc. H2O, and 32.4 cc. Me2CO heated 24 hrs. at 68°, cooled, acidified with 2N HCl, concentrated to 20 cc. at 45°, basified

with saturated aqueous K2CO3, and extracted with CHCl3, and the residue from the extract
chromatographed on Al2O3 yielded 100 mg. substance which gave the picrate of IIIa, m. 145-50° and then 167-9° (EtOH), 110 mg. oil which yielded the picrate of XIII, m. 278-81° (EtOH) [free base m. 72-8° (petr. ether)], and 110 mg. oily C13H17NO (XVII); picrate m. 186-8° (EtOH); HCl salt m. 157-8° (decomposition)
(iso-PrOH-Et2O). I.HCl (4 g.), 5.94 g. Et3N, 40 cc. H2O, and 40 cc. Me2CO refluxed 42 hrs., cooled, acidified with 2N HCl, concentrated to 30 cc., basified with saturated aqueous K2CO3, and extracted with Et2O, and the oily residue
(3.1 g.) from the extract chromatographed on Al2O3 gave 103 mg. III, 210 mg. XIII, and 56 mg. XVII. I.HCl (1.3 g.) treated in the usual manner with K2CO3, the free base stirred 24 hrs. at room temperature in 100 cc. 60% aqueous Me2CO with 2 equivs. Ag2O, refluxed 24 hrs., filtered through Celite, acidified with 2N HCl, concentrated to 20 cc., basified with saturated aqueous K2CO3,
and extracted with CHCl3, and the oily residue from the extract distilled gave 510
mg. yellow oil, b0.01 90-110°, which chromatographed on Al2O3 yielded 147 mg. III, 89 mg. XIII, and 155 mg. oily XVII.

IT 34286-16-3P, 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester
RL: PREP (Preparation)
(preparation of)

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



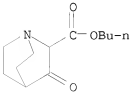
L9 ANSWER 155 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:410798 CAPLUS
DOCUMENT NUMBER: 57:10798
ORIGINAL REFERENCE NO.: 57:2192e-i
TITLE: Synthesis of 2,3-quinuclidinedicarboxylic acid
AUTHOR(S): Mikhlina, E. E.; Rubtsov, M. V.; Vorob'eva, V. Ya.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem.-Pharm. Res. Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1961), 31, 3251-5
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:10798

AB cf. CA 54, 9945i. Azeotropic removal of H2O from 69.3 g. KOH, 11. BuOH, and 100 ml. MePh, evaporation of the residue, and treatment with 120 g. 1-carbethoxymethyl-4-carbethoxypiperidine 5 hr. in MePh gave a viscous mass containing K salt of the enol of Bu 3-oxoquinuclidine-2-carboxylate, which treated with 10% AcOH followed by K2CO3 gave 43.5% Bu 3-oxo-quinuclidine-2-carboxylate, b0.6 137° m. 88°; HCl salt m. 163°. The latter treated with aqueous KCN at 5° gave 68.5% cyanohydrin, m. 107°. Similarly was prepared the cyanohydrin of the Et ester, m. 124-5°. This refluxed 25 hrs. with AcOH-HCl then esterified with EtOH-HCl gave some 3-quinuclidone, separated by sublimation, and 30% di-Et 3-hydroxyquinuclidine-2,3-dicarboxylate (I), b1.2 142°, m. 104-5°, also formed from the corresponding Bu ester cyanohydrin. Refluxing the di-Et ester with 1:1 HCl 5 hrs. gave 65% 3-hydroxyquinuclidine-2,3-dicarboxylic acid-HCl, decomposed at 126°. I with SOCl2 30 hrs. followed by aqueous K2CO3 gave 74.5% di-Et Δ2-dehydroquinuclidine-2,3-dicarboxylate, b0.5 130°; HCl salt m. 148.5°. This refluxed 5 hrs. with 1:1 HCl gave 99% Δ2-dehydroquinuclidine-2,3-dicarboxylic acid, decomposed at 240°; HCl salt, hygroscopic crystals, hydrolyzed by H2O. Hydrogenation over Pt gave quinuclidine-2,3-dicarboxylic acid-HCl, decomposed at 138°, which refluxed 5 hrs. with EtOH-HCl gave the di-Et ester (II), b0.4 115°, which with LiAlH4 gave 58% 2,3-bis(hydroxymethyl)quinuclidine, b0.3 150°; HCl salt, hygroscopic crystals. This and AcCl in refluxing CHCl3 5 hrs. gave 70% diacetate, b0.6 138-40°. II kept 7 days in H2O gave 83.5% 3-carbethoxyquinuclidine-2-carboxylic acid, decomposed at 188-9°.

IT 91554-81-3P, 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester, hydrochloride 91554-82-4P, 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester
RL: PREP (Preparation)
(preparation of)

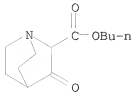
RN 91554-81-3 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 91554-82-4 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester (7CI) (CA INDEX NAME)

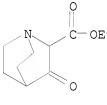


L9 ANSWER 156 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:50470 CAPLUS
DOCUMENT NUMBER: 54:50470
ORIGINAL REFERENCE NO.: 54:9945i,9946a-c
TITLE: Amino acids of the quinuclidine series
AUTHOR(S): Yakhontov, L. N.; Rubtsov, M. V.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Research Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 2343-8
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:50470

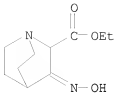
AB Keeping 1.1 g. 2-formylquinuclidine and 0.9 g. EtO2CCH2CN in 3 ml. pyridine with 5 drops piperidine 10 days gave a precipitate of 97.2% Et β-(2-quinuclidyl)-α-cyano-acrylate, m. 139.5-41° (picrate, m. 130.5-10°), which hydrogenated over Pt to α-aminomethyl-β-(2-quinuclidyl)propionic acid, isolated as dipicrate, decomposing 125°; the acid was isolated after the original reaction mixture was hydrogenated and then refluxed with concentrated HCl. Keeping an aqueous solution of Na salt of enol form of Et β-(2-quinuclidyl)-β-oxopropionate 1 day gave Na β-(2-quinuclidyl)-β-oxopropionate, decomposing 240°; this with HONH2 gave 93% β-(2-quinuclidyl)-β-oxopropionic acid oxime, an oil; di-HCl salt, decompose 284°; picrate, m. 167-70°. Hydrogenation of the oxime over Pt gave 78% β-(2-quinuclidyl)-β-aminopropionic acid isolated as di-HCl salt, decomposing 283°. To KOEt in dry MePh was added at 120° 1-carbethoxymethylisonipecotinic acid, the whole was refluxed 5 hrs., cooled, the precipitated K salt of Et 3-oxo-2-quinuclidinecarboxylate was separated and treated with dilute AcOH, yielding 75%
Et 3-oxo-2-quinuclidinecarboxylate, m. 109-10°. This with HONH2.HCl in EtOH gave 80% corresponding oxime, isolated as HCl salt, decomposing 196°. This, hydrogenated over Pt to 99.4% Et 3-amino-2-quinuclidinecarboxylate di-HCl salt, decomposing 185°. This heated with concentrated HCl 6 hrs. gave 91% 3-amino 2-quinuclidinecarboxylic acid di-HCl salt, decomposing 242°.

IT 34286-16-3 110056-51-4 117342-57-1
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

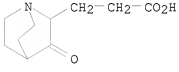


RN 110056-51-4 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester, oxime, hydrochloride (6CI) (CA INDEX NAME)

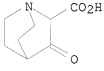


● HCl

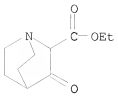
RN 117342-57-1 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



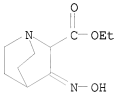
IT 857019-15-9, 2-Quinuclidinecarboxylic acid, 3-oxo-
(derivs.)
RN 857019-15-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo- (CA INDEX NAME)



L9 ANSWER 157 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:50469 CAPLUS
DOCUMENT NUMBER: 54:50469
ORIGINAL REFERENCE NO.: 54:9945d-i
TITLE: Phenanthryl substituted barbiturates
AUTHOR(S): Giannini, M.; Fedi, M.; Russo, F.
CORPORATE SOURCE: Lab. chim. farm. A. Menarini, Florence
SOURCE: Bollettino Chimico Farmaceutico (1959), 98, 714-21
CODEN: BCFAAI; ISSN: 0006-6648
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Refluxing 2.26 g. 9-(chloromethyl)phenanthrene (I) with 62 ml. PrOH, adding 1.42 g. 5-methylbarbituric acid and 0.8 g. HCO2Na in 7 ml. H2O, refluxing 7 hrs., distilling the PrOH to a small volume, mixing the residue with 100 ml. H2O, filtering, and washing with C6H6 until the product was colorless, gave 0.8 g. 5-(9-phenanthrylmethyl)-5-methylbarbituric acid, m. 233-5° (MePh). Refluxing 2.26 g. I in 62 ml. PrOH with 1.56 g. ethylbarbituric acid and 0.8 g. AcONa in 7 ml. H2O for 5 hrs., distilling the solvent, taking up with 100 ml. H2O, allowing to stand, and washing with C6H6 gave 1.2 g. 5-(9-phenanthrylmethyl)-5-ethylbarbituric acid (II), m. 237-8° (xylene). By an analogous procedure there were prepared the following analogs of II: 5-Pr, m. 240° (MePh); 5-Bu, m. 245-8° (MePh and C6H6); 5-allyl, m. 228-30° (xylene). Adding to 6.3 g. K2Cr2O7 in 19 g. H2SO4 and 31 ml. H2O at water bath temperature 2 l g. I, adding later 6.3 g. K2Cr2O7, heating to boiling, cooling, diluting with H2O, washing thoroughly, digesting the solid with NaHSO3 solution at 50-60°, precipitating the phenanthrenequinone with dilute H2SO4 and subliming gave the pure quinone, m. 204°. Treating this quinone in EtOH with o-phenylenediamine gave the corresponding phenazine, m. 217°. Refluxing 2 g. II 48 hrs. with 20 ml. 25% NaOH solution and 20 ml. EtOH, diluting with H2O, acidifying with 10% H2SO4, keeping for crystallization, filtering, dissolving with NaHCO3 solution, precipitating with H2SO4, dissolving in Et2O, and precipitating with petr. ether gave 0.5 g. ethyl-(9-phenanthrylmethyl)malonic acid, m. 152-4° (decomposition). Refluxing 2.26 g. I with 1.58 g. 5-methyl-2-thiobarbituric acid in 60 ml. PrOH to dissoln., adding 0.8 g. NaOAc in 7 ml. H2O, refluxing 1 hr., distilling the PrOH to a small volume, adding 100 ml. H2O, washing the crystals with C6H6, dissolving repeatedly in NaOH and precipitating with HCl gave 2.15 g. 5-(9-phenanthrylmethyl)-5-methyl-2-thiobarbituric acid, m. 280-2°. By an analogous procedure with 0.1 mole material were prepared 3.4 g. 5-Et analog., 250-3° (xylene), 2.5 g. Pr analog. m. 230-1° (xylene), 0.8 g. Bu analog, m. 210° (xylene), and 0.8 g. allyl analog m. 185-9°(MePh). Dissolving 7.4 g. Na in 135 anhydrous EtOH, adding 8.5 g. thiourea and 20 g. di-Et allylmalonate, refluxing 4 hrs., dissolving the precipitate in a min. volume of H2O, and precipitating with HCl gave 3.52 g. 5-allyl-2-thiobarbituric acid, m. 120-2° (xylene). By the same method was prepared from 11.5 g. thiourea and 25 g. di-Et propylmalonate 5.37 g. 5-propyl-2-thiobarbituric acid, m. 163-5° (H2O).
IT 34286-16-3 110056-51-4 117342-57-1
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

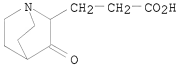


RN 110056-51-4 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester, oxime, hydrochloride (6CI) (CA INDEX NAME)



● HCl

RN 117342-57-1 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



L9 ANSWER 158 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1959:122172 CAPLUS
DOCUMENT NUMBER: 53:122172
ORIGINAL REFERENCE NO.: 53:21953f-i,21954a-c
TITLE: Cyanoethylation of 3-quinuclidinone
AUTHOR(S): Mikhlina, E. E.; Rubtsov, M. V.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Sci. Research Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 118-24
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

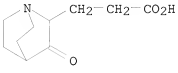
AB Na (24 g.) in 100 ml. MePh and 36 ml. absolute EtOH heated to 120-5°, treated over 1 hr. with 60 g. 1-carbethoxymethyl-4-carbethoxypiperidine in 150 ml. MePh, refluxed 5 hrs., treated with 200 ml. concentrated HCl, the mixture stirred 0.5 hr., the organic layer separated, reextd. with 200 ml. concentrated HCl twice, the acid exts. combined, refluxed 15 hrs., decolorized, and the residue evaporated, treated with 50% KOH, and extracted with C6H6 gave 84.6% 3-quinuclidinone, m. 136-8°; picrate, m. 210°. This (25 g.) in 115 ml. dry dioxane and 3.8 ml. 30% KOH in MeOH heated to 60°, treated over 0.5 hr. with 90 ml. CH2:CHCN, stirred 4 hrs. at 60°, the amorphous polymer filtered off, the filtrate freed of dioxane in vacuo, the residue treated with 100 ml. C6H6, extracted with 50 ml. 10% HCl, and the acid extract treated with K2CO3, and extracted with C6H6 yielded on distillation 14.3 g. 3-quinuclidinone. The distillation residue with 20 ml. absolute EtOH and 1 ml. dry C6H6 yielded 4 g. 3-oxo-2,2-bis(2-cyanoethyl)quinuclidine (Ia), m. 120-2° (EtOH); the mother liquor gave 0.7 g. 3-oxo-2-(2-cyanoethyl)quinuclidine (I), b0.3 121-2°. The same products were formed in Me3COH with MeOH-KOH catalyst. Refluxing I with HCl-AcOH 20 hrs. gave crude 3-oxo-2-(2-carboxyethyl)quinuclidine HCl salt, which, heated 3 hrs. with 9% alc.-dry HCl gave 60.6% 3-oxo-2-(2-carbethoxyethyl)quinuclidine (II), b0.4 136-8°, after the usual treatment of the mixture with K2CO3; the ester refluxed 4 hrs. with 17% HCl gave 96.5% 3-oxo-2-(2-carboxyethyl)quinuclidine HCl salt, decompose 191-3° (EtOH). Heating 0.3 g. II and 1.8 ml. N2H4.H2O with 0.4 g. Na in 9 ml. absolute EtOH in a sealed tube 14 hrs. at 170-80°, distilling the EtOH, refluxing the residue 4 hrs. with 10 ml. H2O, acidifying with HCl, evaporating, heating the residue with 10 ml. 10% alc. HCl 3 hrs., distilling the EtOH, treating the residue with K2CO3, and extracting with Et2O gave 0.17 g. 2-(2-carbethoxyethyl)quinuclidine, b0.2 90-2°, which, refluxed 4 hrs. with 17% HCl, gave 0.06 g. 2-(2-carboxyethyl)quinuclidine HCl salt, decompose 216.5-17.5°. Reduction of II with LiAlH4 in Et2O gave 56.7% 3-hydroxy-2-(3-hydroxypropyl)quinuclidine, b0.4 163-5°; HCl salt, m. 132-3°. Refluxing Ia with AcOH-concentrated HCl 17 hrs. gave 92% 3-oxo-2,2-bis(2-carboxyethyl)quinuclidine HCl salt, decompose 245° (90% EtOH). This refluxed 4 hrs. with 9% alc. HCl gave 63.6% 3-oxo-2,2-bis(2-carbethoxyethyl)quinuclidine (III), b1 190°, m. 58-61°; HCl salt, m. 169-71° (EtOH). Reductions of III with LiAlH4 in Et2O gave 85% 3-hydroxy-2,2-bis(3-hydroxypropyl)quinuclidine, hygroscopic crystals; HCl salt, m. 221-3° (EtOH). Keeping 0.35 g. III with 0.6 ml. N2H4.H2O in 2 ml. absolute EtOH 8 days gave 0.2 g. III dihydrazide, hygroscopic solid yielding a picrate, decompose 168°. Heating III with N2H4.H2O in EtOH-EtONa, as above, 14 hrs. at 160-70° gave 50% 2,2-bis(2-carbethoxyethyl)quinuclidine, b0.2 175-80°, which, refluxed 4 hrs. with 17% HCl, gave 30% 2,2-bis(2-carboxyethyl)quinuclidine HCl salt, decompose 215-18° (Me2CO-EtOH). Heating 1.2 g. LiAlH4, 1 g. Ia, 45 ml. C6H6, and 20 ml. absolute Et2O 40 hrs. at 65-70°, adding 3 ml. H2O, separating the inorg.

salts, washing these with dry pyridine, and evaporating the filtrate gave 59.6% 3-hydroxy-2,2-bis-(2-cyanoethyl)quinuclidine, m. 179-80° (absolute EtOH).

IT 75208-48-9 105339-98-8 105339-99-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 75208-48-9 CAPLUS

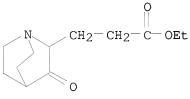
CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, 3-oxo-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 105339-98-8 CAPLUS

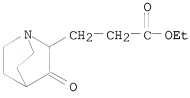
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester, hydrochloride (6CI) (CA INDEX NAME)



● HCl

RN 105339-99-9 CAPLUS

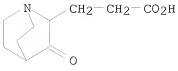
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester (6CI) (CA INDEX NAME)



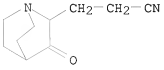
IT 117342-57-1, 2-Quinuclidinepropionic acid, 3-oxo-
(derivs.)

RN 117342-57-1 CAPLUS

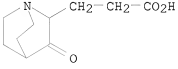
CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



IT 99169-54-7P, 2-Quinuclidinepropionitrile, 3-oxo-
RL: PREP (Preparation)
(preparation of)
RN 99169-54-7 CAPLUS
CN 2-Quinuclidinepropionitrile, 3-oxo- (6CI) (CA INDEX NAME)

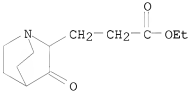


L9 ANSWER 159 OF 160 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1959:122171 CAPLUS
DOCUMENT NUMBER: 53:122171
ORIGINAL REFERENCE NO.: 53:21953e-f
TITLE: Syntheses in the allo-lupinane series. IV. An alternative synthesis of 4-hydroxymethylquinolizidine
AUTHOR(S): Lukes, R.; Vesely, Z.
CORPORATE SOURCE: Vysoka skola chem. technol., Prague
SOURCE: Collection of Czechoslovak Chemical Communications (1959), 24, 2318-23
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: German
AB See C.A. 53, 368f.
IT 75208-48-9 105339-98-8 105339-99-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 75208-48-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, 3-oxo-, hydrochloride (9CI) (CA INDEX NAME)



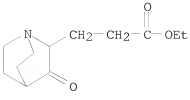
● HCl

RN 105339-98-8 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester, hydrochloride (6CI) (CA INDEX NAME)



● HCl

RN 105339-99-9 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester (6CI) (CA INDEX NAME)



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=> s l9 and cancer
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         53250 CANCERS
        375482 CANCER
                  (CANCER OR CANCERS)
L10           4 L9 AND CANCER

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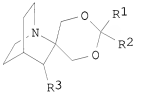
L10 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:590850 CAPLUS
DOCUMENT NUMBER: 147:2004
TITLE: Quinuclidinone derivatives as anticancer agents
INVENTOR(S): Bergmeier, Stephen C.; Evans, Susan C.
PATENT ASSIGNEE(S): Ohio University, USA
SOURCE: PCT Int. Appl., 21pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007062030	A2	20070531	WO 2006-US45045	20061121
WO 2007062030	A3	20080124		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-738673P P 20051121
OTHER SOURCE(S): MARPAT 147:2004
GI

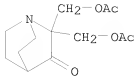


I

AB The invention discloses compds. I (R1, R2 = H, halo, alkyl, cycloalkyl, haloalkyl, aryl, etc.; R3 = O, OH), as well as derivs., metabolites, and prodrugs thereof. Also provided are methods for preparing the quinuclidinone analogs. Further provided are methods for treating, preventing, or delaying the onset of a cancer in a subject in need of such treatment by administering a an effective amount of I, or a derivative, metabolite, or prodrug thereof, to a subject diagnosed with cancer or at risk of developing cancer.

IT 865293-04-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(quinuclidinone derivative anticancer agents)

RN 865293-04-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)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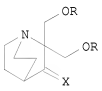
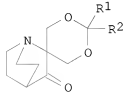
L10 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:87882 CAPLUS
DOCUMENT NUMBER: 144:331585
TITLE: Structure-activity studies of quinuclidinone analogs as anti-proliferative agents in lung cancer cell lines
AUTHOR(S): Malki, Ahmed; Pulipaka, Aravinda B.; Evans, Susan C.; Bergmeier, Stephen C.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Ohio University, Athens, OH, 45701, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(5), 1156-1159
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:331585
GI

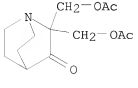


I



II

AB Novel quinuclidinone analogs, such as I [R = H, COMe, X = :O; R = H, X = H,OH] and II [R1 = H, R2 = Ph, (CH2)2Ph, C6H3-3,4-Cl2, C6H4-4-OMe; R1 = R2 = Me; R1R2 = -(CH2)5-], were prepared and assayed for their effects on H1299 lung cancer cell lines alone or with γ-radiation. Two series of quinuclidinone analogs were found to as anti-cancer agents. Of these, four interesting analogs significantly decreased cell viability in H1299 lung cancer cell lines. Two derivs. decreased cell proliferation in a dose-dependent fashion alone or in the presence of γ-radiation. Radiosensitization increased when derivative treatment preceded radiation treatment for both derivs. These preliminary studies show an evidence for both additive and synergistic cytotoxicity for treatment of lung cancer by these novel quinuclidinone analogs.
IT 865293-04-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and structure-activity studies of quinuclidinone analogs as anti-proliferative agents in lung cancer cell lines)
RN 865293-04-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)

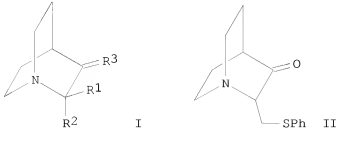


REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1042241 CAPLUS
DOCUMENT NUMBER: 143:326494
TITLE: Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
INVENTOR(S): Westman, Jacob; Wiman, Klas; Selivanova, Galina; Bykov, Vladimir
PATENT ASSIGNEE(S): Aprea AB, Swed.
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090341	A1	20050929	WO 2005-SE412	20050322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223728	A1	20050929	AU 2005-223728	20050322
CA 2552855	A1	20050929	CA 2005-2552855	20050322
EP 1727817	A1	20061206	EP 2005-722253	20050322
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007530534	T	20071101	JP 2007-504913	20050322
US 20070142370	A1	20070621	US 2006-590054	20060821
IN 2006DN05903	A	20070713	IN 2006-DN5903	20061010

PRIORITY APPLN. INFO.: SE 2004-708 A 20040322
WO 2005-SE412 W 20050322
OTHER SOURCE(S): CASREACT 143:326494; MARPAT 143:326494
GI

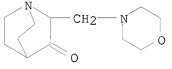


AB Azabicyclooctan-3-ones of formula I [R1, R2 = H, (substituted) CH2OH, acyloxymethyl, etc.; R1R2 = cyclic carbonate, etc.; R33 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative

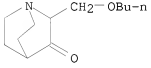
diseases, e.g. cancer as well as autoimmune diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of II against WST-1 assay 3 μM.

IT 41971-48-6P 343954-19-8P 586390-57-0P
865293-03-4P 865293-04-5P 865293-05-6P
865293-06-7P 865293-07-8P 865293-08-9P
865293-09-0P 865293-10-3P 865293-11-4P
865293-12-5P 865293-14-7P 865293-15-8P
865293-16-9P 865293-17-0P 865293-18-1P
865293-19-2P 865293-20-5P 865293-21-6P
865293-22-7P 865293-23-8P 865293-24-9P
865293-26-1P 865293-27-2P 865293-28-3P
865293-29-4P 865293-30-7P 865293-31-8P
865293-32-9P 865293-33-0P 865293-34-1P
865293-35-2P 865293-36-3P 865293-37-4P
865293-38-5P 865293-39-6P 865293-40-9P
865293-41-0P 865293-42-1P 865293-43-2P
865293-44-3P 865293-45-4P 865293-46-5P
865293-47-6P 865293-48-7P 865293-50-1P
865293-51-2P 865293-52-3P 865293-53-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

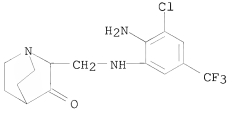
RN 41971-48-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



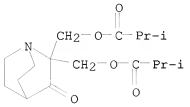
RN 343954-19-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(butoxymethyl)- (CA INDEX NAME)



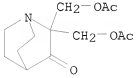
RN 586390-57-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-amino-3-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



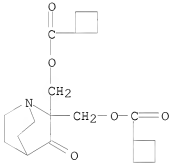
RN 865293-03-4 CAPLUS
CN Propanoic acid, 2-methyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



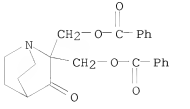
RN 865293-04-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



RN 865293-05-6 CAPLUS
CN Cyclobutanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

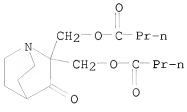


RN 865293-06-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(benzoyloxy)methyl]- (CA INDEX NAME)

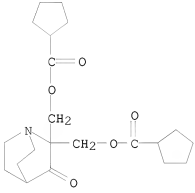


RN 865293-07-8 CAPLUS
CN Butanoic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)

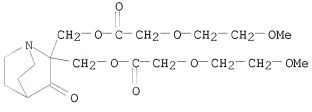
ester (9CI) (CA INDEX NAME)



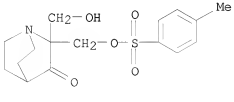
RN 865293-08-9 CAPLUS
CN Cyclopentanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



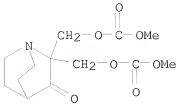
RN 865293-09-0 CAPLUS
CN Acetic acid, (2-methoxyethoxy)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



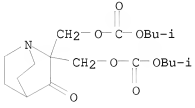
RN 865293-10-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



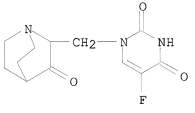
RN 865293-11-4 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) dimethyl ester (9CI) (CA INDEX NAME)



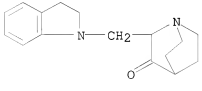
RN 865293-12-5 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)



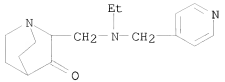
RN 865293-14-7 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]- (CA INDEX NAME)



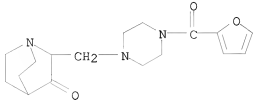
RN 865293-15-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(2,3-dihydro-1H-indol-1-yl)methyl]- (CA INDEX NAME)



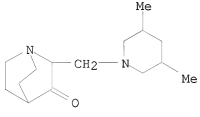
RN 865293-16-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[ethyl(4-pyridinylmethyl)amino]methyl]- (CA INDEX NAME)



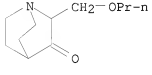
RN 865293-17-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-(2-furanylcarbonyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



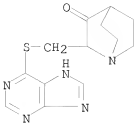
RN 865293-18-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,5-dimethyl-1-piperidinyl)methyl]- (CA INDEX NAME)



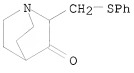
RN 865293-19-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(propoxymethyl)- (CA INDEX NAME)



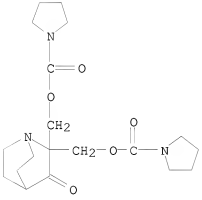
RN 865293-20-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(9H-purin-6-ylthio)methyl]- (CA INDEX NAME)



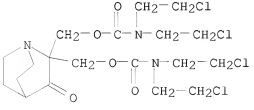
RN 865293-21-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylthio)methyl]- (CA INDEX NAME)



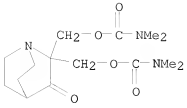
RN 865293-22-7 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



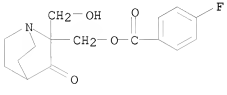
RN 865293-23-8 CAPLUS
CN Carbamic acid, bis(2-chloroethyl)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



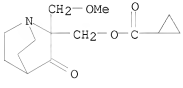
RN 865293-24-9 CAPLUS
CN Carbamic acid, dimethyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



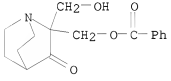
RN 865293-26-1 CAPLUS
CN Benzoic acid, 4-fluoro-, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



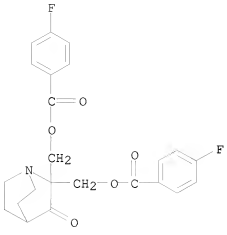
RN 865293-27-2 CAPLUS
CN Cyclopropanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



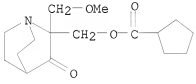
RN 865293-28-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(benzoyloxy)methyl]-2-(hydroxymethyl)- (CA INDEX NAME)



RN 865293-29-4 CAPLUS
CN Benzoic acid, 4-fluoro-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

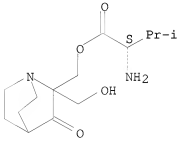


RN 865293-30-7 CAPLUS
CN Cyclopentanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

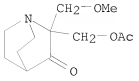


RN 865293-31-8 CAPLUS
CN L-Valine, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

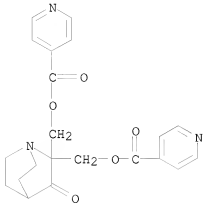
Absolute stereochemistry.



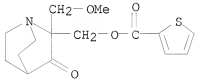
RN 865293-32-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(acetyloxy)methyl]-2-(methoxymethyl)- (CA INDEX NAME)



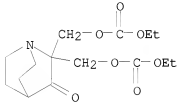
RN 865293-33-0 CAPLUS
CN 4-Pyridinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



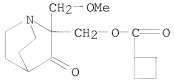
RN 865293-34-1 CAPLUS
CN 2-Thiophenecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-35-2 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) diethyl ester (9CI) (CA INDEX NAME)

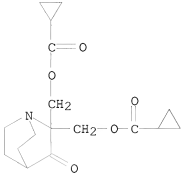


RN 865293-36-3 CAPLUS
CN Cyclobutanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

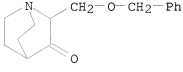


RN 865293-37-4 CAPLUS

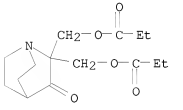
CN Cyclopropanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



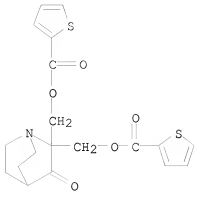
RN 865293-38-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylmethoxy)methyl]- (CA INDEX NAME)



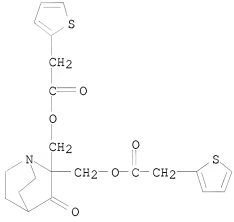
RN 865293-39-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(1-oxopropoxy)methyl]- (CA INDEX NAME)



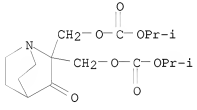
RN 865293-40-9 CAPLUS
CN 2-Thiophenecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



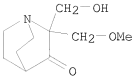
RN 865293-41-0 CAPLUS
CN 2-Thiopheneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-42-1 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 865293-43-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

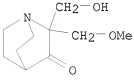


● HCl

RN 865293-44-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, benzoate (1:1) (CA INDEX NAME)

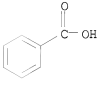
CM 1

CRN 5291-32-7
CMF C10 H17 N O3

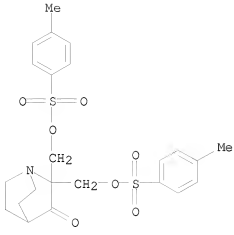


CM 2

CRN 65-85-0
CMF C7 H6 O2



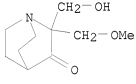
RN 865293-45-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



RN 865293-46-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

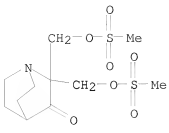
CRN 5291-32-7
CMF C10 H17 N O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

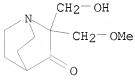
RN 865293-47-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(methylsulfonyl)oxy]methyl]- (CA INDEX NAME)



RN 865293-48-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7
CMF C10 H17 N O3



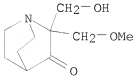
CM 2

CRN 64-19-7
CMF C2 H4 O2

RN 865293-50-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, 4-methylbenzenesulfonate (1:1) (CA INDEX NAME)

CM 1

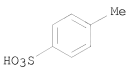
CRN 5291-32-7
CMF C10 H17 N O3



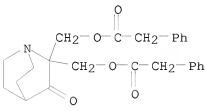
CM 2

CRN 104-15-4

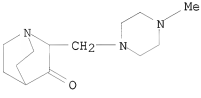
CMF C7 H8 O3 S



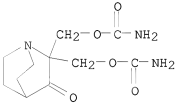
RN 865293-51-2 CAPLUS
CN Benzeneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



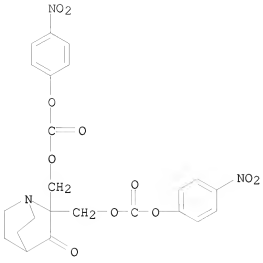
RN 865293-52-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-methyl-1-piperazinyl)methyl]- (CA INDEX NAME)



RN 865293-53-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(aminocarbonyl)oxy]methyl]- (CA INDEX NAME)



IT 865293-25-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)
RN 865293-25-0 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:240769 CAPLUS
DOCUMENT NUMBER: 136:257232
TITLE: 1-azabicyclo[2.2.2]octan-3-one derivatives and maleimide derivatives and their use for treating cancer tumors
INVENTOR(S): Bykov, Vladimir; Selivanova, Galina; Wiman, Klas
PATENT ASSIGNEE(S): Karolinska Innovations AB, Swed.
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002024692	A1	20020328	WO 2001-SE2008	20010919
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2423192	A1	20020328	CA 2001-2423192	20010919
AU 2001090422	A	20020402	AU 2001-90422	20010919
EP 1319000	A1	20030618	EP 2001-970421	20010919
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004509890	T	20040402	JP 2002-529102	20010919
AU 2001290422	B2	20060615	AU 2001-290422	20010919
US 20030166674	A1	20030904	US 2003-381011	20030320
US 6921765	B2	20050726		
US 20050090540	A1	20050428	US 2004-10430	20041214
US 7348330	B2	20080325		

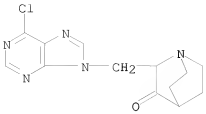
PRIORITY APPLN. INFO.:		US 2000-234164P	P 20000920
		WO 2001-SE2008	W 20010919
		US 2003-381011	A3 20030320

OTHER SOURCE(S): MARPAT 136:257232

AB 1-(Propoxymethyl)maleimide, 2,2-bis(hydroxymethyl)-1-azabicyclo[2,2,2]octan-3-one, and 4 analogs selected based on structure-activity relationship studies are able to reactivate the apoptosis-inducing function of mutant p53 proteins. This reactivation is provided by restoration of sequence-specific DNA-binding activity and transcriptional transactivation function to mutant p53 proteins, and modulation of the conformation-dependent epitopes of the p53 protein. Accordingly, the substances according to the invention will be used in pharmaceutical compns. and methods for treatment of patients suffering from various types of tumors.

IT 405096-63-1
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antitumor azabicycloctanone derivs. and maleimide derivs. reactivate apoptosis-inducing function of mutant p53 proteins)

RN 405096-63-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(6-chloro-9H-purin-9-yl)methyl]- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> s l9 and autoimmun?
         64433 AUTOIMMUN?
L11          2 L9 AND AUTOIMMUN?

=> d ibib abs hittr tot
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The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
information will be displayed in the same order as the format
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specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):kwic

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
AB . . . etc.; R33 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative diseases, e.g. cancer as well as autoimmune diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of. . .
ST quinuclidinone deriv prepn cancer autoimmune heart treatment; azabicyclooctanone prepn cancer autoimmune heart treatment
IT Antitumor agents
Autoimmune disease
Cardiovascular agents
Combination chemotherapy
Heart, disease
Human
Neoplasm
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)
IT Alkaloids, preparation
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(quinuclidinone; preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)
IT 148-82-3, Melphalan 15663-27-1, Cisplatin 25316-40-9, Adriamycin
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(co-drug; preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)
IT 41971-48-6P 343954-19-8P 586390-57-0P
865293-03-4P 865293-04-5P 865293-05-6P
865293-06-7P 865293-07-8P 865293-08-9P
865293-09-0P 865293-10-3P 865293-11-4P
865293-12-5P 865293-13-6P 865293-14-7P
865293-15-8P 865293-16-9P 865293-17-0P
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865293-34-1P 865293-35-2P 865293-36-3P
865293-37-4P 865293-38-5P 865293-39-6P
865293-40-9P 865293-41-0P 865293-42-1P
865293-43-2P 865293-44-3P 865293-45-4P
865293-46-5P 865293-47-6P 865293-48-7P
865293-50-1P 865293-51-2P 865293-52-3P
865293-53-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)
IT 50-44-2, 6-Mercaptopurine 51-21-8, 5-Fluorouracil 71-23-8, Propanol, reactions 79-30-1, Isobutyryl chloride 98-88-4, Benzoyl chloride 100-79-8, Solketal 108-98-5, Thiophenol, reactions 141-75-3, Butyryl chloride 496-15-1, Indoline 543-27-1, Isobutyl chloroformate 1193-65-3, 3-Quinuclidinone hydrochloride 4524-93-0, Cyclopentanecarbonyl chloride 5006-22-4, Cyclobutanecarbonyl chloride 5291-26-9, 2-Methylene-3-quinuclidinone 5832-54-2 16024-55-8, 2-(2-Methoxyethoxy)acetyl chloride 33403-97-3, N-(4-Pyridylmethyl)ethylamine 35794-11-7, 3,5-Dimethylpiperidine 40172-95-0, 1-(2-Furoyl)piperazine

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

IT 79-44-7P 123-75-1P, Pyrrolidine, preparation 821-48-7P, Bis(2-chloroethyl)amine hydrochloride 5608-24-2P 7693-46-1P, 4-Nitrophenyl chloroformate 865293-25-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

AB . . . disorders, which are characterized by an alteration in normal neurotransmission, are also disclosed. Also disclosed are methods for treating inflammation, autoimmune disorders, pain and excess neovascularization, such as that associated with tumor growth.

IT Alzheimer's disease
Anxiety
Autoimmune disease
Central nervous system, disease
Hyperkinesia
Inflammation
Neoplasm
Pain
Parkinson's disease
Schizophrenia
Sepsis
(medicaments; preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes exhibiting activity at nicotinic acetylcholine receptors)

IT 273748-51-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of; preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes exhibiting activity at nicotinic acetylcholine receptors)

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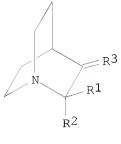
L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1042241 CAPLUS
DOCUMENT NUMBER: 143:326494
TITLE: Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
INVENTOR(S): Westman, Jacob; Wiman, Klas; Selivanova, Galina; Bykov, Vladimir
PATENT ASSIGNEE(S): Aprea AB, Swed.
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090341	A1	20050929	WO 2005-SE412	20050322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223728	A1	20050929	AU 2005-223728	20050322
CA 2552855	A1	20050929	CA 2005-2552855	20050322
EP 1727817	A1	20061206	EP 2005-722253	20050322
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007530534	T	20071101	JP 2007-504913	20050322
US 20070142370	A1	20070621	US 2006-590054	20060821
IN 2006DN05903	A	20070713	IN 2006-DN5903	20061010

PRIORITY APPLN. INFO.: SE 2004-708 A 20040322
WO 2005-SE412 W 20050322
OTHER SOURCE(S): CASREACT 143:326494; MARPAT 143:326494
GI



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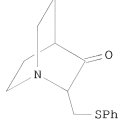


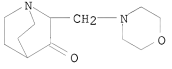
II

AB Azabicyclooctan-3-ones of formula I [R1, R2 = H, (substituted) CH2OH, acyloxymethyl, etc.; R1R2 = cyclic carbonate, etc.; R33 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative

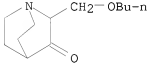
diseases, e.g. cancer as well as autoimmune diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of II against WST-1 assay 3 μM.

IT 41971-48-6P 343954-19-8P 586390-57-0P
865293-03-4P 865293-04-5P 865293-05-6P
865293-06-7P 865293-07-8P 865293-08-9P
865293-09-0P 865293-10-3P 865293-11-4P
865293-12-5P 865293-14-7P 865293-15-8P
865293-16-9P 865293-17-0P 865293-18-1P
865293-19-2P 865293-20-5P 865293-21-6P
865293-22-7P 865293-23-8P 865293-24-9P
865293-26-1P 865293-27-2P 865293-28-3P
865293-29-4P 865293-30-7P 865293-31-8P
865293-32-9P 865293-33-0P 865293-34-1P
865293-35-2P 865293-36-3P 865293-37-4P
865293-38-5P 865293-39-6P 865293-40-9P
865293-41-0P 865293-42-1P 865293-43-2P
865293-44-3P 865293-45-4P 865293-46-5P
865293-47-6P 865293-48-7P 865293-50-1P
865293-51-2P 865293-52-3P 865293-53-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

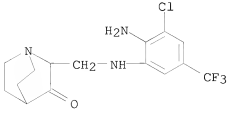
RN 41971-48-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



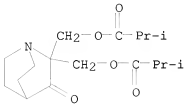
RN 343954-19-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(butoxymethyl)- (CA INDEX NAME)



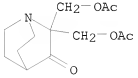
RN 586390-57-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-amino-3-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



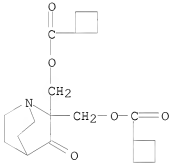
RN 865293-03-4 CAPLUS
CN Propanoic acid, 2-methyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



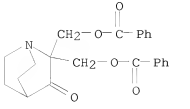
RN 865293-04-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



RN 865293-05-6 CAPLUS
CN Cyclobutanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

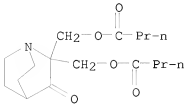


RN 865293-06-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(benzoyloxy)methyl]- (CA INDEX NAME)

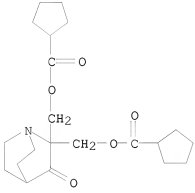


RN 865293-07-8 CAPLUS
CN Butanoic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)

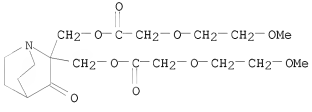
ester (9CI) (CA INDEX NAME)



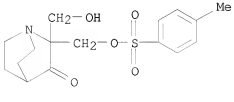
RN 865293-08-9 CAPLUS
CN Cyclopentanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



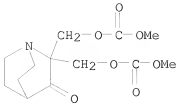
RN 865293-09-0 CAPLUS
CN Acetic acid, (2-methoxyethoxy)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



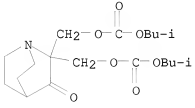
RN 865293-10-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



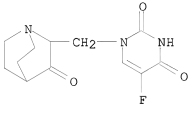
RN 865293-11-4 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) dimethyl ester (9CI) (CA INDEX NAME)



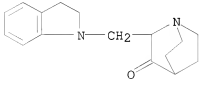
RN 865293-12-5 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)



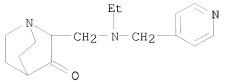
RN 865293-14-7 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]- (CA INDEX NAME)



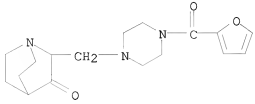
RN 865293-15-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(2,3-dihydro-1H-indol-1-yl)methyl]- (CA INDEX NAME)



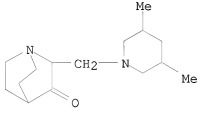
RN 865293-16-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[ethyl(4-pyridinylmethyl)amino]methyl]- (CA INDEX NAME)



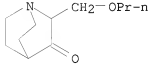
RN 865293-17-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-(2-furanylcarbonyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



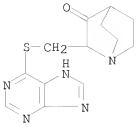
RN 865293-18-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,5-dimethyl-1-piperidinyl)methyl]- (CA INDEX NAME)



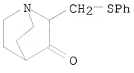
RN 865293-19-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(propoxymethyl)- (CA INDEX NAME)



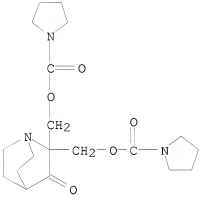
RN 865293-20-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(9H-purin-6-ylthio)methyl]- (CA INDEX NAME)



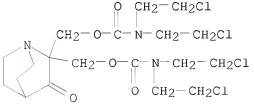
RN 865293-21-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylthio)methyl]- (CA INDEX NAME)



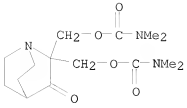
RN 865293-22-7 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



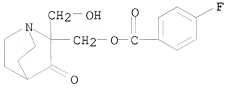
RN 865293-23-8 CAPLUS
CN Carbamic acid, bis(2-chloroethyl)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



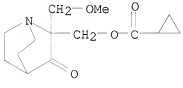
RN 865293-24-9 CAPLUS
CN Carbamic acid, dimethyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



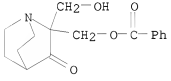
RN 865293-26-1 CAPLUS
CN Benzoic acid, 4-fluoro-, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



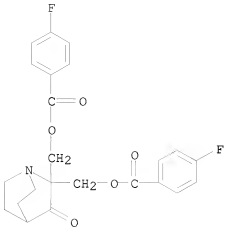
RN 865293-27-2 CAPLUS
CN Cyclopropanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



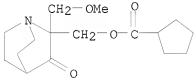
RN 865293-28-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(benzoyloxy)methyl]-2-(hydroxymethyl)- (CA INDEX NAME)



RN 865293-29-4 CAPLUS
CN Benzoic acid, 4-fluoro-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

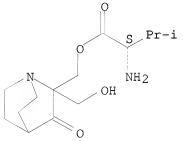


RN 865293-30-7 CAPLUS
CN Cyclopentanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

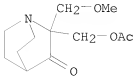


RN 865293-31-8 CAPLUS
CN L-Valine, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

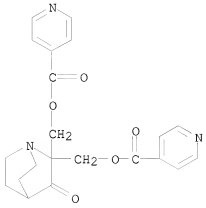
Absolute stereochemistry.



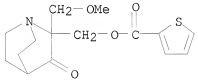
RN 865293-32-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(acetyloxy)methyl]-2-(methoxymethyl)- (CA INDEX NAME)



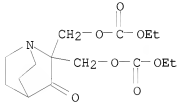
RN 865293-33-0 CAPLUS
CN 4-Pyridinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



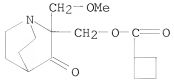
RN 865293-34-1 CAPLUS
CN 2-Thiophenecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-35-2 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) diethyl ester (9CI) (CA INDEX NAME)

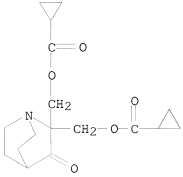


RN 865293-36-3 CAPLUS
CN Cyclobutanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

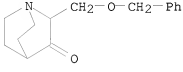


RN 865293-37-4 CAPLUS

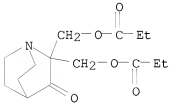
CN Cyclopropanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



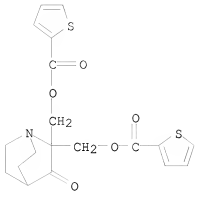
RN 865293-38-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylmethoxy)methyl]- (CA INDEX NAME)



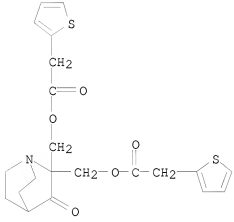
RN 865293-39-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(1-oxopropoxy)methyl]- (CA INDEX NAME)



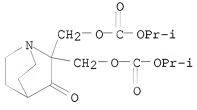
RN 865293-40-9 CAPLUS
CN 2-Thiophenecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



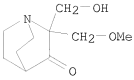
RN 865293-41-0 CAPLUS
CN 2-Thiopheneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-42-1 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 865293-43-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

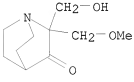


● HCl

RN 865293-44-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, benzoate (1:1) (CA INDEX NAME)

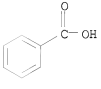
CM 1

CRN 5291-32-7
CMF C10 H17 N O3

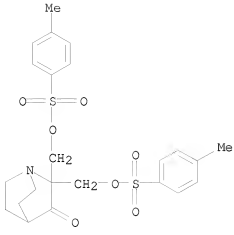


CM 2

CRN 65-85-0
CMF C7 H6 O2



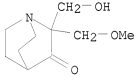
RN 865293-45-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



RN 865293-46-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

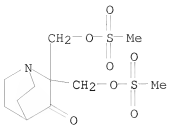
CRN 5291-32-7
CMF C10 H17 N O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

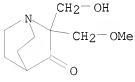
RN 865293-47-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(methylsulfonyl)oxy]methyl]- (CA INDEX NAME)



RN 865293-48-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7
CMF C10 H17 N O3



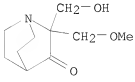
CM 2

CRN 64-19-7
CMF C2 H4 O2

RN 865293-50-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, 4-methylbenzenesulfonate (1:1) (CA INDEX NAME)

CM 1

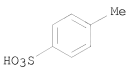
CRN 5291-32-7
CMF C10 H17 N O3



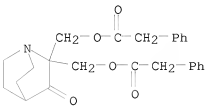
CM 2

CRN 104-15-4

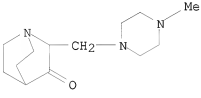
CMF C7 H8 O3 S



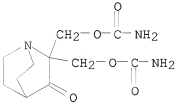
RN 865293-51-2 CAPLUS
CN Benzeneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



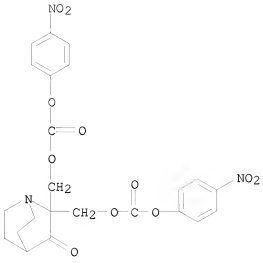
RN 865293-52-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-methyl-1-piperazinyl)methyl]- (CA INDEX NAME)



RN 865293-53-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(aminocarbonyl)oxy]methyl]- (CA INDEX NAME)



IT 865293-25-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)
RN 865293-25-0 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:3665 CAPLUS
DOCUMENT NUMBER: 140:77298
TITLE: Preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes and methods of treatment using these compounds
INVENTOR(S): Mazurov, Anatoly A.; Klucik, Jozef; Miao, Lan; Seamans, Angela S.; Phillips, Teresa Youngpeter; Schmitt, Jeffrey Daniel; Miller, Craig Harrison
PATENT ASSIGNEE(S): Targacept, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 162,129.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040002513	A1	20040101	US 2003-372642	20030221
US 6953855	B2	20051011		
US 6432975	B1	20020813	US 1998-210113	19981211
US 20030045523	A1	20030306	US 2002-162129	20020604
AU 2004215386	A1	20040910	AU 2004-215386	20040220
CA 2514135	A1	20040910	CA 2004-2514135	20040220
WO 2004076449	A2	20040910	WO 2004-US5044	20040220
WO 2004076449	A3	20041216		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1594869	A2	20051116	EP 2004-713356	20040220
EP 1594869	B1	20071219		
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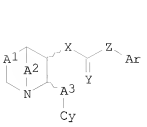
BR 2004007708	A	20060214	BR 2004-7708	20040220
CN 1751041	A	20060322	CN 2004-80004736	20040220
JP 2006518746	T	20060817	JP 2006-503737	20040220
AT 381563	T	20080115	AT 2004-713356	20040220
NZ 541794	A	20080328	NZ 2004-541794	20040220
US 20050255040	A1	20051117	US 2005-157119	20050620
ZA 2005006515	A	20060628	ZA 2005-6515	20050815
MX 2005PA08926	A	20051005	MX 2005-PA8926	20050822
IN 2005KN01718	A	20070323	IN 2005-KN1718	20050829
NO 2005004052	A	20051021	NO 2005-4052	20050831
US 20060247270	A1	20061102	US 2006-458231	20060718

PRIORITY APPLN. INFO.:

US 1998-210113	A1	19981211
US 2002-162129	A2	20020604
US 2003-372642	A	20030221
WO 2004-US5044	A	20040220
US 2005-157119	A1	20050620

OTHER SOURCE(S): MARPAT 140:77298
GI



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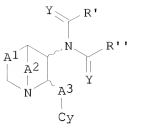


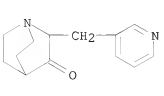
II

AB The present invention relates to 3-substituted-2-(arylalkyl)-1-azabicycloalkanes I [A1 = (CH2)n; A2 = (CH2)m; A3 = (CH2)p; m, n = 1, 2; p = 1 - 4; X = O, NR'; Z = NR', covalent bond, A; A = CR'R'', CR'R''CR'R'', CR':CR', C.tplbond.C (wherein, when Z = bond or A, X = N); Ar = (un)substituted carbocyclic, heterocyclic monocyclic or fused polycyclic aryl; Cy = (un)substituted 5- or 6-membered heteroarom. ring; wavy lines = relative or absolute stereochem. (cis or trans, R or S); R', R'' = H, (un)branched C1-8-alkyl, C3-8-cycloalkyl, heterocyclyl, aryl, arylalkyl {wherein, substituents = alkyl, alkenyl, heterocyclyl, cycloalkyl, (un)substituted aryl, (un)substituted arylalkyl, F, Cl, Br, I, OR', NR'R'', CF3, CN, NO2, C.tplbond.CR', SR', N3, C(:O)NR'R'', NR'C(:O)R'', C(:O)R', C(:O)OR', OC(:O)R', O(CR'R'')rC(:O)R', O(CR'R'')rNR''C(:O)R', O(CR'R'')rNR''SO2R', OC(:O)NR'R'', NR'C(:O)OR'', SO2R', SO2NR'R'', NR'SO2R''}; R'R'' = ring; r = 1 - 6] and II, methods of preparing the compds. and methods of treatment using the compds. The azabicycloalkanes generally are azabicycloheptanes, azabicyclooctanes, or azabicyclononanes. The aryl group in the arylalkyl moiety is a 5- or 6-membered ring heteroarom., preferably 3-pyridinyl and 5-pyrimidinyl moieties, and the alkyl group is typically a C 1-4 alkyl. The substituent at the 3-position of the 1-azabicycloalkane is a carbonyl group-containing moiety, such as an amide, carbamate, urea, thioamide, thiocarbamate, thiourea or similar functionality. The compds. exhibit activity at nicotinic acetylcholine receptors (nAChRs), particularly the α7 nAChR subtype, and are useful towards modulating neurotransmission and the release of ligands involved in neurotransmission. Methods for preventing or treating conditions and disorders, including central nervous system (CNS) disorders, which are characterized by an alteration in normal neurotransmission, are also disclosed. Also disclosed are methods for treating inflammation, autoimmune disorders, pain and excess neovascularization, such as that associated with tumor growth.

IT 273748-51-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of; preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes exhibiting activity at nicotinic acetylcholine receptors)

RN 273748-51-9 CAPLUS

CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(3-pyridinylmethyl)- (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> s l9 and heart
        363973 HEART
         30453 HEARTS
        366123 HEART
                  (HEART OR HEARTS)
L12           2 L9 AND HEART

=> d ibib abs hitstr tot
```
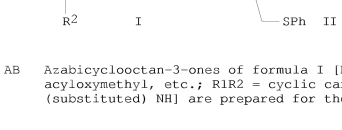

L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1042241 CAPLUS
DOCUMENT NUMBER: 143:326494
TITLE: Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
INVENTOR(S): Westman, Jacob; Wiman, Klas; Selivanova, Galina; Bykov, Vladimir
PATENT ASSIGNEE(S): Aprea AB, Swed.
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090341	A1	20050929	WO 2005-SE412	20050322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223728	A1	20050929	AU 2005-223728	20050322
CA 2552855	A1	20050929	CA 2005-2552855	20050322
EP 1727817	A1	20061206	EP 2005-722253	20050322
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007530534	T	20071101	JP 2007-504913	20050322
US 20070142370	A1	20070621	US 2006-590054	20060821
IN 2006DN05903	A	20070713	IN 2006-DN5903	20061010

PRIORITY APPLN. INFO.: SE 2004-708 A 20040322
WO 2005-SE412 W 20050322
OTHER SOURCE(S): CASREACT 143:326494; MARPAT 143:326494
GI



AB Azabicyclooctan-3-ones of formula I [R1, R2 = H, (substituted) CH2OH, acyloxymethyl, etc.; R1R2 = cyclic carbonate, etc.; R33 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative

diseases, e.g. cancer as well as autoimmune diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of II against WST-1 assay 3 μM.

IT 41971-48-6P 343954-19-8P 586390-57-0P
865293-03-4P 865293-04-5P 865293-05-6P
865293-06-7P 865293-07-8P 865293-08-9P
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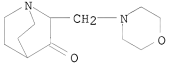
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

RN 41971-48-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



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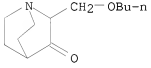
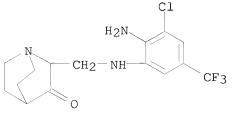
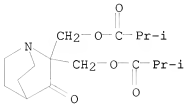


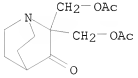
RN 586390-57-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-amino-3-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



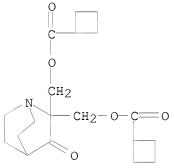
RN 865293-03-4 CAPLUS
CN Propanoic acid, 2-methyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



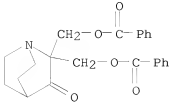
RN 865293-04-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



RN 865293-05-6 CAPLUS
CN Cyclobutanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

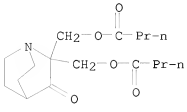


RN 865293-06-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(benzoyloxy)methyl]- (CA INDEX NAME)

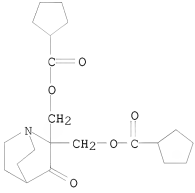


RN 865293-07-8 CAPLUS
CN Butanoic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene)

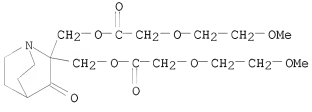
ester (9CI) (CA INDEX NAME)



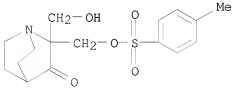
RN 865293-08-9 CAPLUS
CN Cyclopentanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



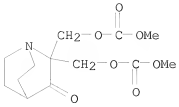
RN 865293-09-0 CAPLUS
CN Acetic acid, (2-methoxyethoxy)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



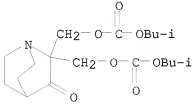
RN 865293-10-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



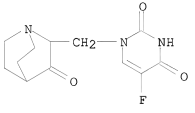
RN 865293-11-4 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) dimethyl ester (9CI) (CA INDEX NAME)



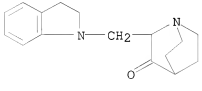
RN 865293-12-5 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)



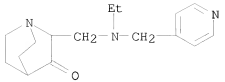
RN 865293-14-7 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]- (CA INDEX NAME)



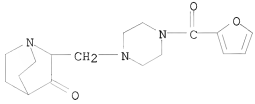
RN 865293-15-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(2,3-dihydro-1H-indol-1-yl)methyl]- (CA INDEX NAME)



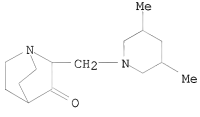
RN 865293-16-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[ethyl(4-pyridinylmethyl)amino]methyl]- (CA INDEX NAME)



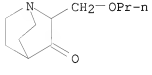
RN 865293-17-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-(2-furanylcarbonyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



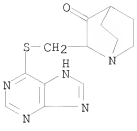
RN 865293-18-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,5-dimethyl-1-piperidinyl)methyl]- (CA INDEX NAME)



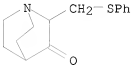
RN 865293-19-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(propoxymethyl)- (CA INDEX NAME)



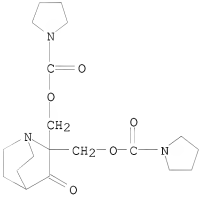
RN 865293-20-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(9H-purin-6-ylthio)methyl]- (CA INDEX NAME)



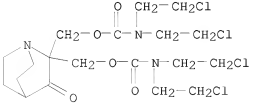
RN 865293-21-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylthio)methyl]- (CA INDEX NAME)



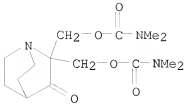
RN 865293-22-7 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



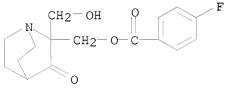
RN 865293-23-8 CAPLUS
CN Carbamic acid, bis(2-chloroethyl)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



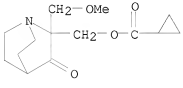
RN 865293-24-9 CAPLUS
CN Carbamic acid, dimethyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



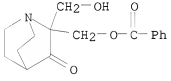
RN 865293-26-1 CAPLUS
CN Benzoic acid, 4-fluoro-, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



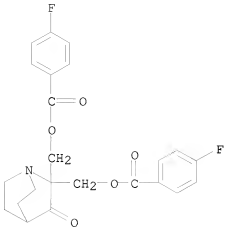
RN 865293-27-2 CAPLUS
CN Cyclopropanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



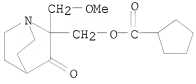
RN 865293-28-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(benzoyloxy)methyl]-2-(hydroxymethyl)- (CA INDEX NAME)



RN 865293-29-4 CAPLUS
CN Benzoic acid, 4-fluoro-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

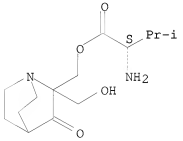


RN 865293-30-7 CAPLUS
CN Cyclopentanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

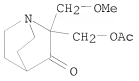


RN 865293-31-8 CAPLUS
CN L-Valine, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

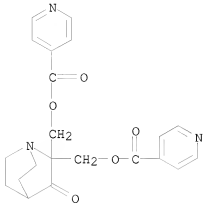
Absolute stereochemistry.



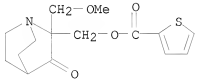
RN 865293-32-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(acetyloxy)methyl]-2-(methoxymethyl)- (CA INDEX NAME)



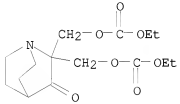
RN 865293-33-0 CAPLUS
CN 4-Pyridinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



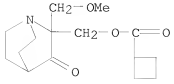
RN 865293-34-1 CAPLUS
CN 2-Thiophenecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-35-2 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) diethyl ester (9CI) (CA INDEX NAME)

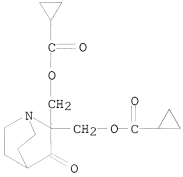


RN 865293-36-3 CAPLUS
CN Cyclobutanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

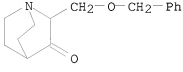


RN 865293-37-4 CAPLUS

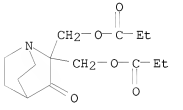
CN Cyclopropanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



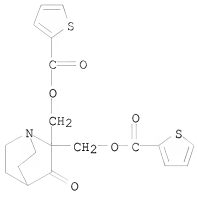
RN 865293-38-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylmethoxy)methyl]- (CA INDEX NAME)



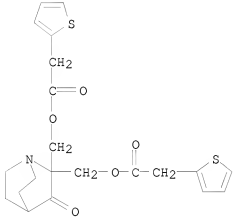
RN 865293-39-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(1-oxopropoxy)methyl]- (CA INDEX NAME)



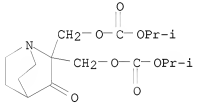
RN 865293-40-9 CAPLUS
CN 2-Thiophenecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



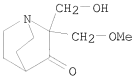
RN 865293-41-0 CAPLUS
CN 2-Thiopheneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-42-1 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 865293-43-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

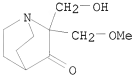


● HCl

RN 865293-44-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, benzoate (1:1) (CA INDEX NAME)

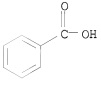
CM 1

CRN 5291-32-7
CMF C10 H17 N O3

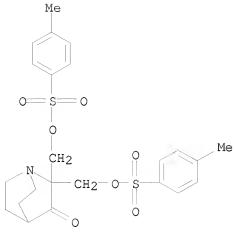


CM 2

CRN 65-85-0
CMF C7 H6 O2



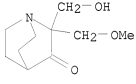
RN 865293-45-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



RN 865293-46-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

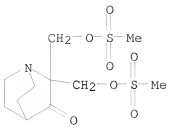
CRN 5291-32-7
CMF C10 H17 N O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

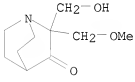
RN 865293-47-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(methylsulfonyl)oxy]methyl]- (CA INDEX NAME)



RN 865293-48-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7
CMF C10 H17 N O3



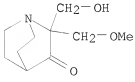
CM 2

CRN 64-19-7
CMF C2 H4 O2

RN 865293-50-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, 4-methylbenzenesulfonate (1:1) (CA INDEX NAME)

CM 1

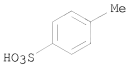
CRN 5291-32-7
CMF C10 H17 N O3



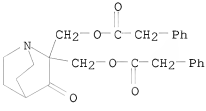
CM 2

CRN 104-15-4

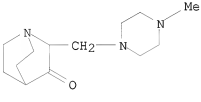
CMF C7 H8 O3 S



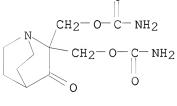
RN 865293-51-2 CAPLUS
CN Benzeneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



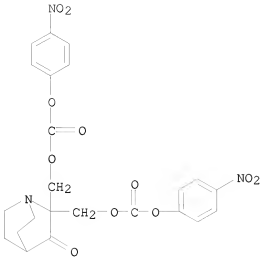
RN 865293-52-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-methyl-1-piperazinyl)methyl]- (CA INDEX NAME)



RN 865293-53-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(aminocarbonyl)oxy]methyl]- (CA INDEX NAME)



IT 865293-25-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)
RN 865293-25-0 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:199680 CAPLUS
DOCUMENT NUMBER: 114:199680
ORIGINAL REFERENCE NO.: 114:33481a,33484a
TITLE: Preparation of renin-inhibitory di-, tri-, and tetrapeptide cardiovascular drug
INVENTOR(S): Greenlee, William J.; Broeke, Jan Ten
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 389127	A1	19900926	EP 1990-302145	19900228
R: CH, DE, FR, GB, IT, LI, NL				
US 5049548	A	19910917	US 1989-319448	19890303
CA 2011327	A1	19900903	CA 1990-2011327	19900302
JP 02300200	A	19901212	JP 1990-51593	19900302

PRIORITY APPLN. INFO.: US 1989-319448 A 19890303
OTHER SOURCE(S): CASREACT 114:199680; MARPAT 114:199680

AB The peptides ABEGTJ [A = (un)substituted heterocyclyl; B = NA1CH[(CH2)mR]CO; E = absent or NA1CH[(CH2)nR1]CO; A1, R = H, alkyl; R1 = H, aryl, etc.; m = 0, 1, 2; n = 1-4; G = HNC[(CH2)mR2]CH(OH)CHR3CO, HNC[(CH2)mR2]CH(OH)CO, etc.; R2 = alkyl, aryl, (un)substituted cycloalkyl; R3 = H, alkyl, alkenyl, etc.; T = absent or NHCH[(CH2)m]RCO; J = Y(CH2)x(CHR3)y(CH2)zR4; Y = O, NH, etc.; R4 = H, OH, alkyl; x, y = 0, 1; Z = 0, 1-4] are prepared as renin inhibitors, useful as drugs for the treatment of hypertension and congestive heart failure (no data). To a solution of 0.09 g 3-quinuclidinone and 4.15 g Phe-O-tert-Bu in 50 mL MeOH was added a solution of 2.95 g Na cyanoborohydride in 13 mL MeOH and 5.78 g pyridine-HCl, to give Nα-(quinuclidine-3(RS)-yl)phenylalanine tert-Bu ester-HCl.

IT 52763-22-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive coupling of, to protected amino acids)

RN 52763-22-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

● HCl

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=> s l9 and hyperproliferative
          1982 HYPERPROLIFERATIVE
L13          1 L9 AND HYPERPROLIFERATIVE

=> d ibib abs hitstr tot
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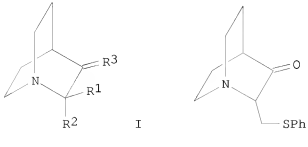
L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1042241 CAPLUS
DOCUMENT NUMBER: 143:326494
TITLE: Preparation of azabicyclooctan-3-one derivatives for the treatment of cancer, autoimmune and heart diseases
INVENTOR(S): Westman, Jacob; Wiman, Klas; Selivanova, Galina; Bykov, Vladimir
PATENT ASSIGNEE(S): Aprea AB, Swed.
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090341	A1	20050929	WO 2005-SE412	20050322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223728	A1	20050929	AU 2005-223728	20050322
CA 2552855	A1	20050929	CA 2005-2552855	20050322
EP 1727817	A1	20061206	EP 2005-722253	20050322
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007530534	T	20071101	JP 2007-504913	20050322
US 20070142370	A1	20070621	US 2006-590054	20060821
IN 2006DN05903	A	20070713	IN 2006-DN5903	20061010

PRIORITY APPLN. INFO.: SE 2004-708 A 20040322
WO 2005-SE412 W 20050322
OTHER SOURCE(S): CASREACT 143:326494; MARPAT 143:326494
GI



AB Azabicyclooctan-3-ones of formula I [R1, R2 = H, (substituted) CH2OH, acyloxymethyl, etc.; R1R2 = cyclic carbonate, etc.; R33 = O, S, (substituted) NH] are prepared for the treatment of hyperproliferative diseases, e.g. cancer as well as autoimmune

diseases and heart diseases. Thus, II was prepared from 2-methylene-3-quinuclidinone hydrochloride and thiophenol in 14% yield. The IC50 value of II against WST-1 assay 3 μM.

IT 41971-48-6P 343954-19-8P 586390-57-0P
865293-03-4P 865293-04-5P 865293-05-6P
865293-06-7P 865293-07-8P 865293-08-9P
865293-09-0P 865293-10-3P 865293-11-4P
865293-12-5P 865293-14-7P 865293-15-8P
865293-16-9P 865293-17-0P 865293-18-1P
865293-19-2P 865293-20-5P 865293-21-6P
865293-22-7P 865293-23-8P 865293-24-9P
865293-26-1P 865293-27-2P 865293-28-3P
865293-29-4P 865293-30-7P 865293-31-8P
865293-32-9P 865293-33-0P 865293-34-1P
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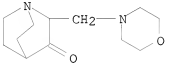
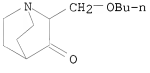
865293-38-5P 865293-39-6P 865293-40-9P
865293-41-0P 865293-42-1P 865293-43-2P
865293-44-3P 865293-45-4P 865293-46-5P
865293-47-6P 865293-48-7P 865293-50-1P
865293-51-2P 865293-52-3P 865293-53-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)

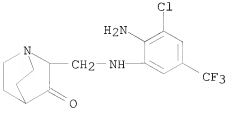
RN 41971-48-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



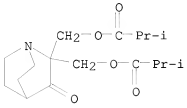
RN 343954-19-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(butoxymethyl)- (CA INDEX NAME)



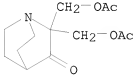
RN 586390-57-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-amino-3-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



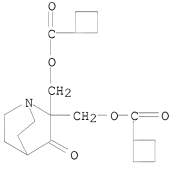
RN 865293-03-4 CAPLUS
CN Propanoic acid, 2-methyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



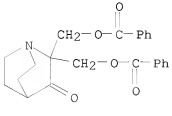
RN 865293-04-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(acetyloxy)methyl]- (9CI) (CA INDEX NAME)



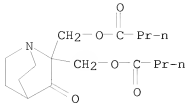
RN 865293-05-6 CAPLUS
CN Cyclobutanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



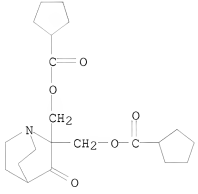
RN 865293-06-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(benzoyloxy)methyl]- (CA INDEX NAME)



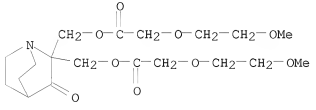
RN 865293-07-8 CAPLUS
CN Butanoic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



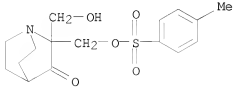
RN 865293-08-9 CAPLUS
CN Cyclopentanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



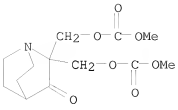
RN 865293-09-0 CAPLUS
CN Acetic acid, (2-methoxyethoxy)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



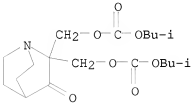
RN 865293-10-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



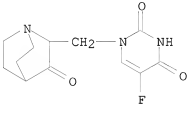
RN 865293-11-4 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) dimethyl ester (9CI) (CA INDEX NAME)



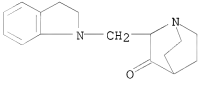
RN 865293-12-5 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)



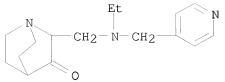
RN 865293-14-7 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]- (CA INDEX NAME)



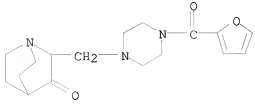
RN 865293-15-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(2,3-dihydro-1H-indol-1-yl)methyl]- (CA INDEX NAME)



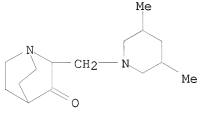
RN 865293-16-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[ethyl(4-pyridinylmethyl)amino]methyl]- (CA INDEX NAME)



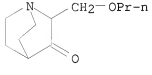
RN 865293-17-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[4-(2-furanylcarbonyl)-1-piperazinyl]methyl]- (CA INDEX NAME)



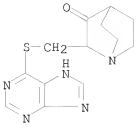
RN 865293-18-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,5-dimethyl-1-piperidinyl)methyl]- (CA INDEX NAME)



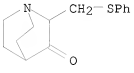
RN 865293-19-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(propoxymethyl)- (CA INDEX NAME)



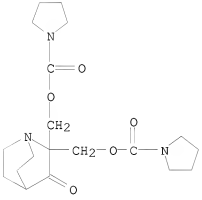
RN 865293-20-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(9H-purin-6-ylthio)methyl]- (CA INDEX NAME)



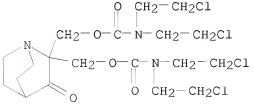
RN 865293-21-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylthio)methyl]- (CA INDEX NAME)



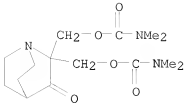
RN 865293-22-7 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



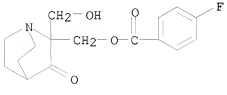
RN 865293-23-8 CAPLUS
CN Carbamic acid, bis(2-chloroethyl)-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



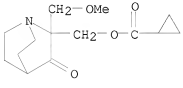
RN 865293-24-9 CAPLUS
CN Carbamic acid, dimethyl-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



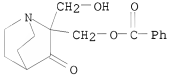
RN 865293-26-1 CAPLUS
CN Benzoic acid, 4-fluoro-, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



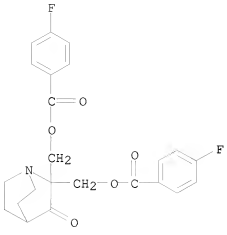
RN 865293-27-2 CAPLUS
CN Cyclopropanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



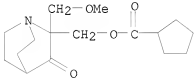
RN 865293-28-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(benzoyloxy)methyl]-2-(hydroxymethyl)- (CA INDEX NAME)



RN 865293-29-4 CAPLUS
CN Benzoic acid, 4-fluoro-, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)

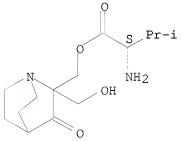


RN 865293-30-7 CAPLUS
CN Cyclopentanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

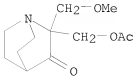


RN 865293-31-8 CAPLUS
CN L-Valine, [2-(hydroxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

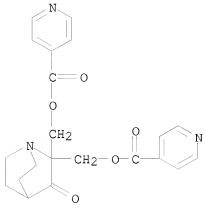
Absolute stereochemistry.



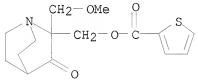
RN 865293-32-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(acetyloxy)methyl]-2-(methoxymethyl)- (CA INDEX NAME)



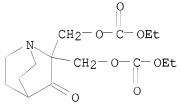
RN 865293-33-0 CAPLUS
CN 4-Pyridinecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



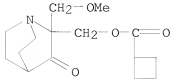
RN 865293-34-1 CAPLUS
CN 2-Thiophenecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)



RN 865293-35-2 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) diethyl ester (9CI) (CA INDEX NAME)

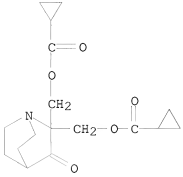


RN 865293-36-3 CAPLUS
CN Cyclobutanecarboxylic acid, [2-(methoxymethyl)-3-oxo-1-azabicyclo[2.2.2]oct-2-yl]methyl ester (CA INDEX NAME)

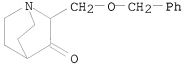


RN 865293-37-4 CAPLUS

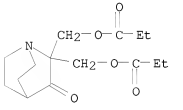
CN Cyclopropanecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



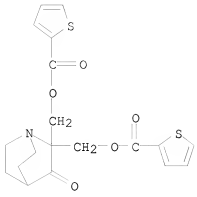
RN 865293-38-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylmethoxy)methyl]- (CA INDEX NAME)



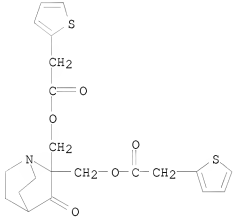
RN 865293-39-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[(1-oxopropoxy)methyl]- (CA INDEX NAME)



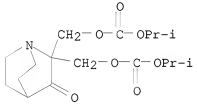
RN 865293-40-9 CAPLUS
CN 2-Thiophenecarboxylic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



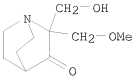
RN 865293-41-0 CAPLUS
CN 2-Thiopheneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



RN 865293-42-1 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 865293-43-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

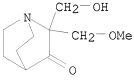


● HCl

RN 865293-44-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, benzoate (1:1) (CA INDEX NAME)

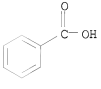
CM 1

CRN 5291-32-7
CMF C10 H17 N O3

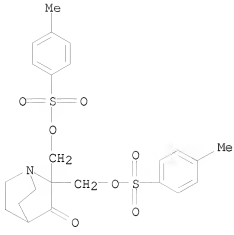


CM 2

CRN 65-85-0
CMF C7 H6 O2



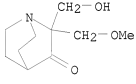
RN 865293-45-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[[(4-methylphenyl)sulfonyl]oxy]methyl]- (CA INDEX NAME)



RN 865293-46-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

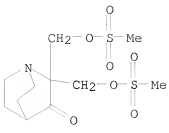
CRN 5291-32-7
CMF C10 H17 N O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

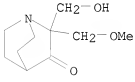
RN 865293-47-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(methylsulfonyl)oxy]methyl]- (CA INDEX NAME)



RN 865293-48-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 5291-32-7
CMF C10 H17 N O3



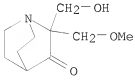
CM 2

CRN 64-19-7
CMF C2 H4 O2

RN 865293-50-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)-, 4-methylbenzenesulfonate (1:1) (CA INDEX NAME)

CM 1

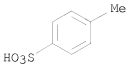
CRN 5291-32-7
CMF C10 H17 N O3



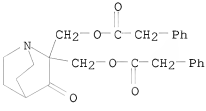
CM 2

CRN 104-15-4

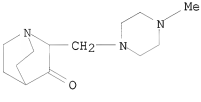
CMF C7 H8 O3 S



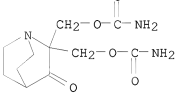
RN 865293-51-2 CAPLUS
CN Benzeneacetic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) ester (9CI) (CA INDEX NAME)



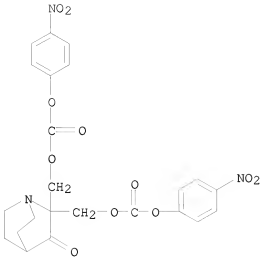
RN 865293-52-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-methyl-1-piperazinyl)methyl]- (CA INDEX NAME)



RN 865293-53-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2-bis[[(aminocarbonyl)oxy]methyl]- (CA INDEX NAME)



IT 865293-25-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinuclidinone derivs. for treatment of cancer, autoimmune and heart diseases)
RN 865293-25-0 CAPLUS
CN Carbonic acid, (3-oxo-1-azabicyclo[2.2.2]oct-2-ylidene)bis(methylene) bis(4-nitrophenyl) ester (9CI) (CA INDEX NAME)



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L15        134 L9 AND PY<2003

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L15 ANSWER 100 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:413478 CAPLUS
DOCUMENT NUMBER: 81:13478
ORIGINAL REFERENCE NO.: 81:2171a,2174a
TITLE: Benzopyrans
INVENTOR(S): Wright, Howard Bernard; Horrom, Bruce W.
PATENT ASSIGNEE(S): Abbott Laboratories
SOURCE: Ger. Offen., 23 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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DE 2351734	A1	19740418	DE 1973-2351734		19731015	<--
US 3915996	A	19751028	US 1973-367027		19730608	<--
CA 992080	A1	19760629	CA 1973-180946		19730913	<--
ZA 7307326	A	19740828	ZA 1973-7326		19730914	<--
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NL 7313595	A	19740418	NL 1973-13595		19731003	<--
JP 49072259	A	19740712	JP 1973-112902		19731009	<--
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NO 141089	B	19791001	NO 1973-4000		19731015	<--
NO 141089	C	19800109				
DK 143029	B	19810316	DK 1973-5575		19731015	<--
DK 143029	C	19811026				
BE 806152	A1	19740416	BE 1973-136757		19731016	<--
CH 591468	A5	19770915	CH 1973-14626		19731016	<--
FI 8100118	A	19810116	FI 1981-118		19810116	<--
PRIORITY APPLN. INFO.:			US 1972-298132	A	19721016	
			US 1973-367027	A	19730608	
			FI 1973-3019	A	19730927	

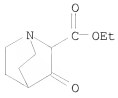
GI For diagram(s), see printed CA Issue.

AB Four benzopyrans [I and II, X = CH2, CH2CH2, or N(CH2C.tplbond.CH)-CH2; R = Me] and (or) their salts with HCl or HBr, useful as analgesics, were prepared by reaction of resorcinols with β-oxo-esters, e.g. III (R1 = CH2Ph) (IV) in MeSO3H to give corresponding I or II (RR = O), followed by reaction with MeMgBr, and optionally hydrogenolytic cleavage of the N-protecting CH2-Ph group. Thus, 3,5-(HO)2C6H3CHMe(CH2)3C6H4F-4 reacted with IV.HCl in MeSO3H in the presence of POCl3 to give I.HCl [X = N(CH2Ph)CH2, RR = O] (V.HCl). V reacted with Me-MgBr in PhOMe to give, after treatment with dilute H2SO4, I [X = N(CH2Ph)CH2, R = Me], which on hydrogenolysis and reaction with HC.tplbond.CCH2Br gave I [X = N(CH2C.tplbond.CH)CH2, R = Me].

IT 52763-22-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with resorcinols)

RN 52763-22-1 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)



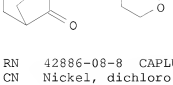
● HCl

L15 ANSWER 101 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:77753 CAPLUS
DOCUMENT NUMBER: 80:77753
ORIGINAL REFERENCE NO.: 80:12485a,12488a
TITLE: Transition metal chemistry of quinuclidinone-containing ligands. II. Spectral and megnetic properties of some transition metal complexes containing 2(N-morpholinylmethyl)-3-quinuclidinone and related ligands
AUTHOR(S): Dickinson, Richard C.; Long, Gary J.
CORPORATE SOURCE: Dep. Chem., Univ. Missouri, Rolla, MO, USA
SOURCE: Inorganic Chemistry (1974), 13(2), 262-9
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Complexes of Co(II), Ni(II), and Fe(II) halides with 2-(N-morpholinyl)methyl-3-quinuclidinone (L) were prepared by adding the appropriate metal salt to the ligand in alc. solns. The complexes have pseudotetrahedral microsymmetry around the central metal ion as indicated by their spectral and magnetic properties; the coordination sphere contains 1 bidentate N-bonded ligand and 2 halide atoms. Ligand field band assignments, metal-halide stretching frequencies, and magnetic susceptibility data are given for each of the complexes. The Co(II) and Ni(II) perchlorate complexes of L were also prepared, and each contains 2 bidentate ligands which provide a tetrahedral ligand field that is stronger than for the halide complexes. The apparent preference of the ligand for 1-to-1 metal-to-ligand coordination and the consequent tetrahedral structures result from a combination of the size of the quinuclidine group and the rigidity of the 5-membered chelate ring formed by the coordinated ligand. In addition to these pseudotetrahedral complexes, an octahedral Ni chloride complex which contains bridging chloride ligands is reported. A cobaltous thiocyanate complex also has an octahedral structure in the solid state and a tetrahedral structure in solution

IT 41971-48-6P 42886-08-8P 42892-78-4P
42892-79-5P 42892-80-8P 42892-81-9P
42892-82-0P 42892-83-1P 42892-84-2P
42892-85-3P 42892-86-4P 42892-87-5P
42942-73-4P 43021-09-6P 54218-39-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

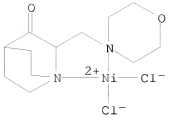
RN 41971-48-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)



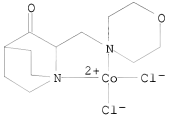
RN 42886-08-8 CAPLUS
CN Nickel, dichloro[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

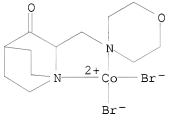
CRN 48175-79-7
CMF C12 H20 C12 N2 Ni O2
CCI CCS



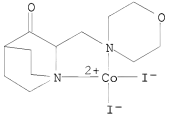
RN 42892-78-4 CAPLUS
CN Cobalt, dichloro[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



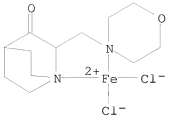
RN 42892-79-5 CAPLUS
CN Cobalt, dibromo[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



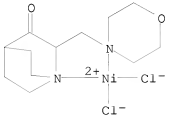
RN 42892-80-8 CAPLUS
CN Cobalt, diiodo[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



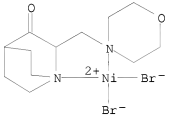
RN 42892-81-9 CAPLUS
CN Iron, dichloro[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



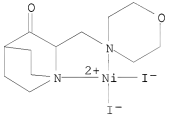
RN 42892-82-0 CAPLUS
CN Nickel, dichloro[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



RN 42892-83-1 CAPLUS
CN Nickel, dibromo[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



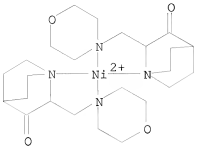
RN 42892-84-2 CAPLUS
CN Nickel, diiodo[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



RN 42892-85-3 CAPLUS
CN Nickel(2+), bis[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

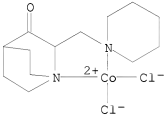
CRN 48228-23-5
CMF C24 H40 N4 Ni O4
CCI CCS



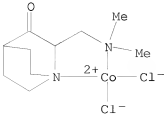
CM 2

CRN 14797-73-0
CMF Cl O4

RN 42892-86-4 CAPLUS
CN Cobalt, dichloro[2-(1-piperidinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)

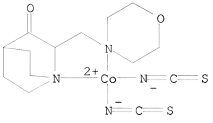


RN 42892-87-5 CAPLUS
CN Cobalt, dichloro[2-[(dimethylamino)methyl]-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)- (9CI) (CA INDEX NAME)



RN 42942-73-4 CAPLUS

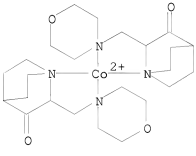
CN Cobalt, [2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



RN 43021-09-6 CAPLUS
CN Cobalt(2+), bis[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]-, (T-4)-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

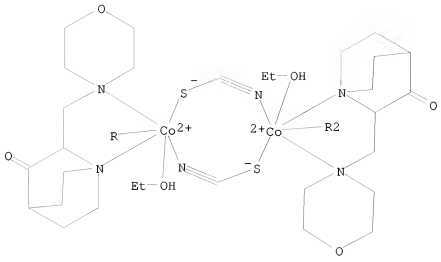
CRN 49857-57-0
CMF C24 H40 Co N4 O4
CCI CCS



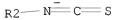
CM 2

CRN 14797-73-0
CMF Cl O4

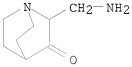
RN 54218-39-2 CAPLUS
CN Cobalt, bis(ethanol)bis[2-(4-morpholinylmethyl)-1-azabicyclo[2.2.2]octan-3-one-N1,N2]bis[μ-(thiocyanato-N:S)]bis(thiocyanato-N)di- (9CI) (CA INDEX NAME)


O
N
S
N
Et
OH
N
O
R
Co
2+
2+
Co
R2
O
N
N
S
N
Et
OH
O


S
C
N
R


R2
N
C
S

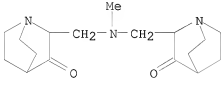
L15 ANSWER 102 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:499990 CAPLUS
DOCUMENT NUMBER: 79:99990
ORIGINAL REFERENCE NO.: 79:16163a,16166a
TITLE: Selected first-row transition metal coordination compounds of 2-(N-aminomethyl)-3-quinuclidinone chelates
AUTHOR(S): Dickinson, Richard C.
CORPORATE SOURCE: Univ. Missouri, Rolla, MO, USA
SOURCE: (1972) 118 pp. Avail.: Univ. Microfilms, Ann Arbor, Mich., Order No. 73-17,062
From: Diss. Abstr. Int. B 1973, 34(1), 116
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 42817-38-9DP, 1-Azabicyclo[2.2.2]octan-3-one, 2-(aminomethyl)-, transition metal complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42817-38-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(aminomethyl)- (CA INDEX NAME)



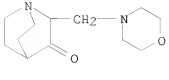
L15 ANSWER 103 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:431939 CAPLUS
DOCUMENT NUMBER: 79:31939
ORIGINAL REFERENCE NO.: 79:5181a,5184a
TITLE: Amine-substituted 2-methylene-3-quinuclidones as antibacterial agents
INVENTOR(S): Elkin, Samuel; Lieberman, Hillel
PATENT ASSIGNEE(S): Temple University
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3726877	A	19730410	US 1970-84927	19701028 <--
PRIORITY APPLN. INFO.:			US 1970-84927 A	19701028

GI For diagram(s), see printed CA Issue.
AB About 30 title compds. (I, R = morpholino, Ph2N, 2-isoquinolinyl, p-ClC6H4NH, o-MeC6H4NH, etc.) were prepared Thus, 2-methylene-3-quinuclidone was treated with morpholine to give I(R = morpholino). Several I were reduced to the corresponding alcs. I were antibacterial against Pseudomonas aeruginosa, Staphylococcus aureus, Escherichia coli, etc.
IT 19576-25-1P 41971-48-6P 41971-49-7P
41971-50-0P 41971-51-1P 41971-52-2P
41971-53-3P 41971-54-4P 41971-55-5P
41971-57-7P 41971-59-9P 41971-60-2P
41971-61-3P 41971-63-5P 41971-64-6P
41971-65-7P 41971-66-8P 41971-67-9P
41971-68-0P 41971-69-1P 41971-70-4P
41971-71-5P 41971-72-6P 41971-73-7P
42036-83-9P 42036-85-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19576-25-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2'-[(methylimino)bis(methylene)]bis- (9CI) (CA INDEX NAME)

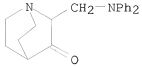


RN 41971-48-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(4-morpholinylmethyl)- (CA INDEX NAME)

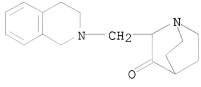


RN 41971-49-7 CAPLUS

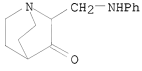
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(diphenylamino)methyl]- (CA INDEX NAME)



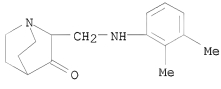
RN 41971-50-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]- (CA INDEX NAME)



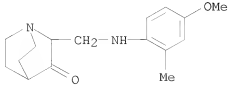
RN 41971-51-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(phenylamino)methyl]- (CA INDEX NAME)



RN 41971-52-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,3-dimethylphenyl)amino]methyl]- (CA INDEX NAME)

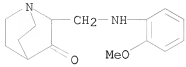


RN 41971-53-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-methoxy-2-methylphenyl)amino]methyl]- (CA INDEX NAME)

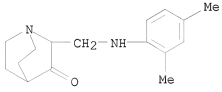


RN 41971-54-4 CAPLUS

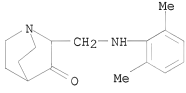
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2-methoxyphenyl)amino]methyl]- (CA INDEX NAME)



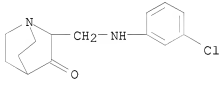
RN 41971-55-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,4-dimethylphenyl)amino]methyl]- (CA INDEX NAME)



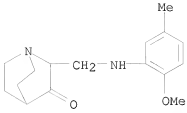
RN 41971-57-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,6-dimethylphenyl)amino]methyl]- (CA INDEX NAME)



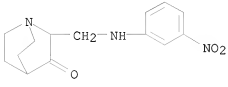
RN 41971-59-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(3-chlorophenyl)amino]methyl]- (CA INDEX NAME)



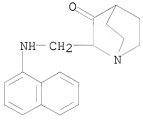
RN 41971-60-2 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2-methoxy-5-methylphenyl)amino]methyl]- (CA INDEX NAME)



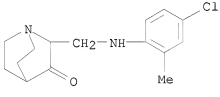
RN 41971-61-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(3-nitrophenyl)amino]methyl]- (CA INDEX NAME)



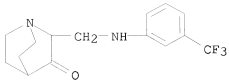
RN 41971-63-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(1-naphthalenylamino)methyl]- (CA INDEX NAME)



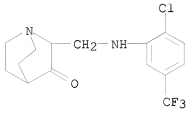
RN 41971-64-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-chloro-2-methylphenyl)amino]methyl]- (CA INDEX NAME)



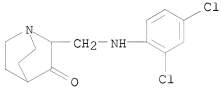
RN 41971-65-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[3-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



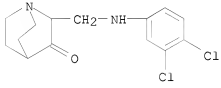
RN 41971-66-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[2-chloro-5-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



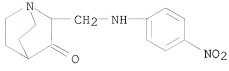
RN 41971-67-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,4-dichlorophenyl)amino]methyl]- (CA INDEX NAME)



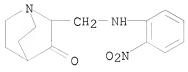
RN 41971-68-0 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(3,4-dichlorophenyl)amino]methyl]- (CA INDEX NAME)



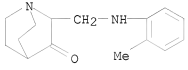
RN 41971-69-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-nitrophenyl)amino]methyl]- (CA INDEX NAME)



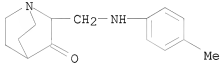
RN 41971-70-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2-nitrophenyl)amino]methyl]- (CA INDEX NAME)



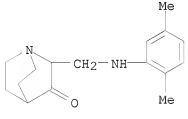
RN 41971-71-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2-methylphenyl)amino]methyl]- (CA INDEX NAME)



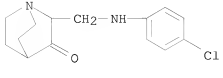
RN 41971-72-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-methylphenyl)amino]methyl]- (CA INDEX NAME)



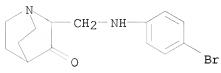
RN 41971-73-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(2,5-dimethylphenyl)amino]methyl]- (CA INDEX NAME)



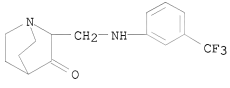
RN 42036-83-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-chlorophenyl)amino]methyl]- (CA INDEX NAME)



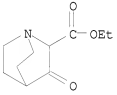
RN 42036-85-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(4-bromophenyl)amino]methyl]- (CA INDEX NAME)



L15 ANSWER 104 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:431727 CAPLUS
DOCUMENT NUMBER: 79:31727
ORIGINAL REFERENCE NO.: 79:5145a,5148a
TITLE: Optically active triptycenes. VI. Optical resolution of 2,5-dihydroxy-8-methoxycarbonyltriptycene and absolute configuration of 2,5-dimethoxy-8-methoxycarbonyltriptycene
AUTHOR(S): Shimizu, Yasumi; Naito, Taketoshi; Ogura, Fumio; Nakagawa, Masazumi
CORPORATE SOURCE: Fac. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(5), 1520-5
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2,5-Dihydroxy-8-(methoxycarbonyl)triptycene (I) was resolved via its dicamphanate derivative The absolute configuration of (+)-2,5-dimethoxy-8-(methoxycarbonyl)triptycene derived from I was (1R,6S) (by chemical correlation with (+)-2,5-dimethoxy-7-(dimethylamino)triptycene-HBr.
IT 41971-65-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41971-65-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[[3-(trifluoromethyl)phenyl]amino]methyl]- (CA INDEX NAME)



L15 ANSWER 105 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:57263 CAPLUS
DOCUMENT NUMBER: 78:57263
ORIGINAL REFERENCE NO.: 78:9087a,9090a
TITLE: Use of mass spectrometry in structural and stereochemical studies. I. Mass spectra of β-quinuclidones and β-benzo(b)quinuclidones
AUTHOR(S): Ermakov, A. I.; Sheinker, Yu. N.; Mikhlina, E. E.; Mastafanova, L. I.; Vorob'eva, V. Ya.; Yanina, A. D.; Yakhontov, L. N.; Kostyanovskii, R. G.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (10), 1404-10
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The mass spectra of β-quinuclidinones (I; R = H, Q = H2, X = O; R = CO2Me, Q = O, X = H2; R = CO2Et, Q = H2, X = O; R = CO2Et, Q = O, X = H2) and benzo[b]quinuclidones (II; R = H, CO2Et) were given. Labeling expts. indicated that fragmentation occurred by rupture of the bridge bond containing the keto group and subsequent loss of CO.
IT 34286-16-3
RL: PRP (Properties)
(mass spectrum of)
RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

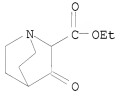


L15 ANSWER 106 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:551126 CAPLUS
DOCUMENT NUMBER: 77:151126
ORIGINAL REFERENCE NO.: 77:24839a,24842a
TITLE: PMR study of the tautomerism of 2-ethoxycarbonyl-3-oxoquinuclidine and -benzo [b] quinuclidine
AUTHOR(S): Turchin, K. F.; Sheinker, Yu. N.; Mikhlina, E. E.; Vorob'eva, V. Ya.; Yanina, A. D.; Yakhontov, L. N.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (7), 978-83
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian

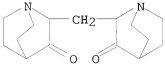
AB 2-Ethoxycarbonyl-3-oxoquinuclidine existed primarily as the keto tautomer in nonpolar solvents, and as the N-protonated enolate in hydroxylic solvents; the lifetime of the individual forms in CD3OD at 75° was .apprx.0.3 sec. 2-Ethoxycarbonyl-3-oxobenzo-[b]quinuclidine existed as a mixture of syn and anti keto tautomers in CDCl3 and in CD3OD, with the syn diastereomer predominating; no enolic tautomers were observed The H at C-2 underwent D exchange in CD3OD at -24° (half life .apprx.2 min, activation energy .apprx.8 kcal/mol).

IT 34286-16-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(tautomerism of, NMR in relation to)

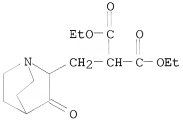
RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



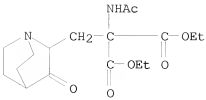
L15 ANSWER 107 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:461774 CAPLUS
DOCUMENT NUMBER: 77:61774
ORIGINAL REFERENCE NO.: 77:10219a,10222a
TITLE: Michael reactions in the quinuclidin-3-one series
AUTHOR(S): Oppenheimer, Edna; Bergmann, Ernst D.
CORPORATE SOURCE: Dep. Chem., Heb. Univ., Jerusalem, Israel
SOURCE: Synthesis (1972), (5), 269-71
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Enamine (I), prepared from 3-quinuclidinone (II, R = R1 = H) (III) and pyrrolidine, underwent Michael reaction with CH2:-CRCOMe (R = H, Me) to give the corresponding ethanoquinolines (IV); III gave II [RR1 = CHR2; R2 = H (V), Ph] with R2CHO, which were treated with (EtO2C)2CH2 in NaOEtHOEt to give II [R = H, R1 = (EtO2C)2CHCHR2; R2 = H (VI), Ph, resp.]. II (RR1 = PhCHMeCH, RR1 = Me2CHCH) were prepared analogously. V gave II [R = H, R1 = (EtO2C)2CHCHR2; R2 = NHAc] (VII) with AcNHCH(CO2Et)2. VI and VII were hydrolyzed with HCl-HOAc to II [R = H, R1 = HO2C(CH2)2; R = H, R1 = HO2CCH(NH2)CH2], resp.
IT 37040-83-8P 37040-87-2P 37040-88-3P
37040-89-4P 37040-90-7P 37395-64-5P
37395-65-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 37040-83-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2'-methylenebis- (CA INDEX NAME)



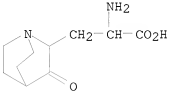
RN 37040-87-2 CAPLUS
CN Propanedioic acid, [(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 37040-88-3 CAPLUS
CN Propanedioic acid, (acetylamino)[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)methyl]-, diethyl ester (9CI) (CA INDEX NAME)

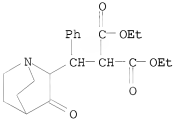


RN 37040-89-4 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, α-amino-3-oxo-, dihydrochloride (9CI) (CA INDEX NAME)

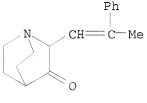


● 2 HCl

RN 37040-90-7 CAPLUS
CN Propanedioic acid, [(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)phenylmethyl]-, diethyl ester (9CI) (CA INDEX NAME)

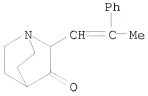


RN 37395-64-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(2-phenyl-1-propenyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 37395-65-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(2-phenyl-1-propenyl)- (9CI) (CA INDEX NAME)

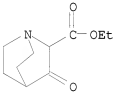


L15 ANSWER 108 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:404638 CAPLUS
DOCUMENT NUMBER: 77:4638
ORIGINAL REFERENCE NO.: 77:830h,831a
TITLE: Tautomerism of 2-ethoxycarbonyl-3-Oxo derivatives of quinuclidine and benzo[b]quinuclidine
AUTHOR(S): Sheinker, Yu. N.; Peresleni, E. M.; Persianova, I. V.; Mikhlina, E. E.; Vorob'eva, V. Ya.; Yanina, A. D.; Yakhontov, L. N.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (2), 229-33
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian

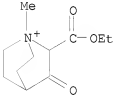
AB Using ir and uv spectroscopy and potentiometric titration existence of 2-ethoxycarbonyl-3-oxoquinuclidine in the keto, enol, and zwitterionic forms was established. The tautomeric equilibrium was affected by the aggregate state (concentration) and by the solvent nature. In the crystalline state and in polar solvents the zwitterionic form prevailed, in nonpolar solvents existence of keto and enol forms was proved. -Ethoxycarbonyl-3-oxobenzo [b]quinuclidine existed in the keto form in al

IT 34286-16-3 37832-15-8
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(tautomerism of, ir spectrum in relation to)

RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



RN 37832-15-8 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 2-(ethoxycarbonyl)-1-methyl-3-oxo-, iodide (9CI) (CA INDEX NAME)



L15 ANSWER 109 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:140119 CAPLUS
DOCUMENT NUMBER: 76:140119
ORIGINAL REFERENCE NO.: 76:22727a,22730a
TITLE: Hydrogen transfer from formyl compounds to α,β-unsaturated ketones catalyzed by ruthenium, rhodium, and iridium complexes
AUTHOR(S): Blum, Jochanan; Sasson, Yoel; Iflah, Shulah
CORPORATE SOURCE: Dep. Org. Chem., Heb. Univ., Jerusalem, Israel
SOURCE: Tetrahedron Letters (1972), (11), 1015-18
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Phenethyl ketones PhCH2CH2COR (I, R = Ph, CMe3 and Me) were prepared by transfer-hydrogenation of PhCH:CHCOR using α-naphthaldehyde, p-MeC6H4CHO, HCONHMe or HCO2H as H donors in the presence of catalytic amts. of (Ph3P)3RuCl2, (Ph3P)3RhCl or (Ph3P)2IrCl(CO). The transferred H atoms are derived exclusively from the formyl group. HCO2H was an excellent H donor and gave 94-6% yields of the ketones. Side reactions due to decarbonylation of the aldehydes and condensation of the ketones were also present. BuPh in 10% yield was obtained by reducing PhCH2CH2CH:CH2 with HCO2H.

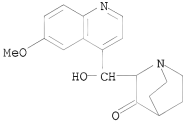
IT 5291-14-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 5291-14-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-methyl- (CA INDEX NAME)

L15 ANSWER 110 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:46360 CAPLUS
DOCUMENT NUMBER: 76:46360
ORIGINAL REFERENCE NO.: 76:7480h,7481a
TITLE: Synthetic quinine analogs. V. Quinolinemethanols related to devinylquinine
AUTHOR(S): Bender, D. R.; Coffen, D. L.
CORPORATE SOURCE: Dep. Chem., Univ. Colorado, Boulder, CO, USA
SOURCE: Journal of Heterocyclic Chemistry (1971), 8(6), 937-42
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 76:46360

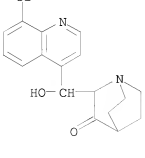
AB Aldol condensation of quin-olinecarboxaldehydes with 3-quinuclidinone followed by acid-catalyzed hydration of the resulting α,β-unsatd. ketones provides a short and versatile synthesis of devinylquinine derivs. A novel rearrangement of 2-(9-phenanthrylmethylene)-3-quinuclidinyl carbinols leading to dibenzindole derivs. is described.

IT 35722-03-3P 35839-90-8P 35839-91-9P
35845-49-9P 35845-54-6P 35870-57-6P
35870-58-7P 36468-36-7P 36547-75-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

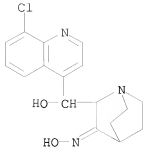
RN 35722-03-3 CAPLUS
CN 10,11-Dinorcinchonan-7-one, 9-hydroxy-6'-methoxy-, (8α)-(±)-(9CI) (CA INDEX NAME)



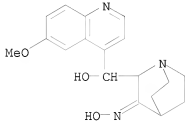
RN 35839-90-8 CAPLUS
CN 10,11-Dinorcinchonan-7-one, 8'-chloro-9-hydroxy-, (8α)-(±)- (9CI) (CA INDEX NAME)



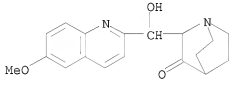
RN 35839-91-9 CAPLUS
CN 10,11-Dinorcinchonan-7-one, 8'-chloro-9-hydroxy-, oxime, (8α)-(±)- (9CI) (CA INDEX NAME)



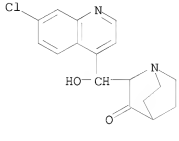
RN 35845-49-9 CAPLUS
CN 10,11-Dinorcinchonan-7-one, 9-hydroxy-6'-methoxy-, oxime,
(8α)-(±)- (9CI) (CA INDEX NAME)



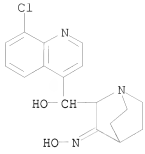
RN 35845-54-6 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[hydroxy(6-methoxy-2-quinolinyl)methyl]-
(CA INDEX NAME)



RN 35870-57-6 CAPLUS
CN 10,11-Dinorcinchonan-7-one, 7'-chloro-9-hydroxy-, (8α)-(±)- (9CI)
(CA INDEX NAME)

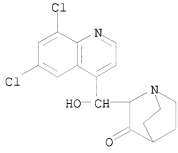


RN 35870-58-7 CAPLUS
CN 10,11-Dinorcinchonan-7-one, 8'-chloro-9-hydroxy-, oxime, hydrochloride,
(8α)-(±)- (9CI) (CA INDEX NAME)

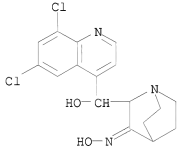


● x HCl

RN 36468-36-7 CAPLUS
CN 10,11-Dinorcinchonan-7-one, 6',8'-dichloro-9-hydroxy-, (8α)-(±)-
(9CI) (CA INDEX NAME)

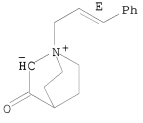


RN 36547-75-8 CAPLUS
CN 10,11-Dinorcinchonan-7-one, 6',8'-dichloro-9-hydroxy-, oxime,
(8α)-(±)- (9CI) (CA INDEX NAME)

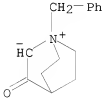


L15 ANSWER 111 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:45521 CAPLUS
DOCUMENT NUMBER: 76:45521
ORIGINAL REFERENCE NO.: 76:7349a,7352a
TITLE: Effect of transition-state geometry on the [2,3]-sigmatropic rearrangements of ammonium ylides
AUTHOR(S): Mageswaran, S.; Ollis, W. D.; Sutherland, I. O.; Thebtaranonth, Y.
CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, UK
SOURCE: Journal of the Chemical Society [Section] D: Chemical Communications (1971), (22), 1494-5
CODEN: CCJDAO; ISSN: 0577-6171
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The ylides (I, R=PhCH2, PhCH:-CHCH2) prepared from 1-benzyl- and 1-(cinnamyl)-1-azoniabicyclo[2.2.2]octan-3-one bromides by treatment with aqueous NaOH did not undergo [2,3]-sigmatropic rearrangements cleanly but gave complex mixts. of products. The less strained ylide (II, R=PhCH:CHCH2) generated by base from a 1-(cinnamyl)-1-azoniabicyclo[3.3.1]nonan-3-one salt gave at 120° 85% of the [2,3]-sigmatropically rearranged product, 2-(1-phenyl-2-propenyl)-1-azabicyclo[3.3.1]nonan-3-one.
IT 79841-03-5 79841-04-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrolysis of)
RN 79841-03-5 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-oxo-1-(3-phenyl-2-propenyl)-, ylide, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 79841-04-6 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-oxo-1-(phenylmethyl)-, ylide (9CI) (CA INDEX NAME)

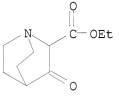


L15 ANSWER 112 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:551255 CAPLUS
DOCUMENT NUMBER: 75:151255
ORIGINAL REFERENCE NO.: 75:23853a,23856a
TITLE: Stereochemistry of benzo[b]quinuclidines. I. Determination of the configuration of 3- and 2,3-substituted benzo[b]quinuclidines by PMR
AUTHOR(S): Turchin, K. F.; Mikhlina, E. E.; Yanina, A. D.; Vorob'eva, V. Ya.; Yakhontov, L. N.; Sheinker, Yu. N.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1971), 7(7), 981-6
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian

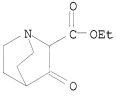
AB Observed trends in changes of chemical shifts and spin–spin coupling consts. of the quinuclidine unit protons owing to substitution in 2- and 3-positions of benzo[b]quinuclidine permit determination of syn and anti orientations (to the attached benzene ring) of protons in 2- and 3-positions in the title compds.

IT 34286-16-3
RL: PRP (Properties)
(nuclear magnetic resonance of)

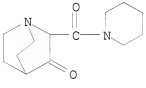
RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



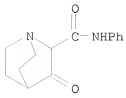
L15 ANSWER 113 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:550911 CAPLUS
DOCUMENT NUMBER: 75:150911
ORIGINAL REFERENCE NO.: 75:23801a,23804a
TITLE: Mass spectra of β-quinuclidones and β-benzoquinuclidones
AUTHOR(S): Ermakov, A. I.; Sheinker, Yu. N.; Mikhlina, E. E.; Mastafanova, L. I.; Vorob'eva, V. Ya.; Yanina, A. D.; Yakhnotov, L. N.; Kostyanovskii, R. G.
CORPORATE SOURCE: S. Ordzhonikidze All Union Chem.-Pharm. Res. Inst., Moscow, USSR
SOURCE: Organic Mass Spectrometry (1971), 5(9), 1029-41
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mass spectra of quinuclid-3-one, benzoquinuclid-3-one, 2-azaquinuclid-3-one, 2-azabenzoquinuclid-3-one and some of their functional substituted derivs. were investigated. Fragmentation of the compds. investigated proceeded through the open form of the mol. ion with cleavage of a bridgehead bond containing the carbonyl group and subsequent elimination of CO.
IT 34286-16-3 34291-64-0 34291-65-1
34291-66-2
RL: PRP (Properties)
(mass spectrum of)
RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



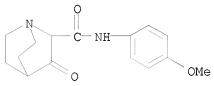
RN 34291-64-0 CAPLUS
CN Piperidine, 1-[(3-oxo-1-azabicyclo[2.2.2]oct-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



RN 34291-65-1 CAPLUS
CN 2-Quinuclidinecarboxanilide, 3-oxo- (8CI) (CA INDEX NAME)



RN 34291-66-2 CAPLUS
CN 2-Quinuclidinecarbox-p-anisidide, 3-oxo- (8CI) (CA INDEX NAME)



L15 ANSWER 114 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:510339 CAPLUS
DOCUMENT NUMBER: 75:110339
ORIGINAL REFERENCE NO.: 75:17427a,17430a
TITLE: 2-[N-(o-alkoxyphenyl)piperazinomethyl]-3-quinuclidinones as tranquilizers and central nervous system depressants in mammals
INVENTOR(S): Biel, John H.; Hopps, Harvey B.
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

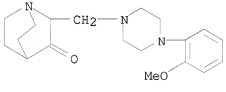
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3598825	A	19710810	US 1967-690087	19671213 <--
PRIORITY APPLN. INFO.:			US 1967-690087 A	19671213

GI For diagram(s), see printed CA Issue.

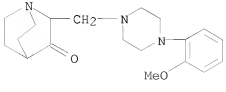
AB The substituted quinuclidinones (I, R = lower alkyl) are prepared by reacting an N-(o-alkoxyphenyl)piperazine with 2-methylene-3-quinuclidinone (II) in a suitable solvent at 20-100°. Mannich reaction of 3-quinuclidinone with Me2NH and CH2O in absolute alc. and heating the Mannich base intermediate at reflux temperature yields II by spontaneous deamination. Thus, II and N-(o-methoxyphenyl)piperazine in MeOH kept 60 hr at 20° yielded 63% I (R = Me), m. 108.5-9.5°. Similarly were obtained I (R = Et, Pr, iso-Pr, Bu, CMe3, C5H11).

IT 33606-15-4P 33606-16-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 33606-15-4 CAPLUS
CN 3-Quinuclidinone, 2-[[4-(o-methoxyphenyl)-1-piperazinyl]methyl]- (8CI) (CA INDEX NAME)



RN 33606-16-5 CAPLUS
CN 3-Quinuclidinone, 2-[[4-(o-methoxyphenyl)-1-piperazinyl]methyl]-, trihydrochloride (8CI) (CA INDEX NAME)

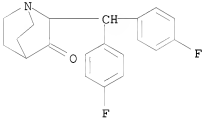


●3 HCl

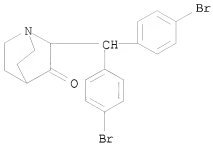
L15 ANSWER 115 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:405735 CAPLUS
DOCUMENT NUMBER: 75:5735
ORIGINAL REFERENCE NO.: 75:951a,954a
TITLE: 2-Benzhydrylquinuclidines as diuretics
INVENTOR(S): Warawa, Edward J.
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3560510	A	19710202	US 1969-804691	19690305 <--
PRIORITY APPLN. INFO.:			US 1969-804691 A	19690305

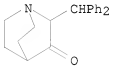
GI For diagram(s), see printed CA Issue.
AB Cis and trans isomers of the title compds. are obtained by isolating the cis or trans isomer from a mixture of cis,trans-2-benzhydryl-3-(benzylamino)quinuclidines by chromatog. and subsequent catalytic debenzylation. Alternatively, a mixture of cis,trans-3-amino analog is acetylated with Ac2O and the 3-acetamido derivs. separated by fractional crystallization from iso-PrOH and hydrolyzed in concentrated HCl. BzH reacted with 3-quinuclidinone in alc. in the presence of a base, the 2-benzylidene-3-quinuclidinone treated with PhMgBr in Et2O-C6H6, the resultant 2-benzhydryl-3-quinuclidinone distilled azeotropically with PhCH2NH2 in PhMe in the presence of p-MeC6H4SO3H, and the 2-benzhydryl-3-(benzylimino)quinuclidine reduced with NaBH4 yielded pure cis-I.
IT 24802-69-5P 24802-70-8P 32531-66-1P
32531-67-2P 32531-68-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24802-69-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[bis(4-fluorophenyl)methyl]- (CA INDEX NAME)



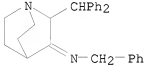
RN 24802-70-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[bis(4-bromophenyl)methyl]- (CA INDEX NAME)



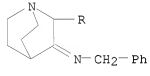
RN 32531-66-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(diphenylmethyl)- (CA INDEX NAME)

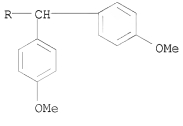


RN 32531-67-2 CAPLUS
CN Benzenemethanamine, N-[2-(diphenylmethyl)-1-azabicyclo[2.2.2]oct-3-ylidene]- (CA INDEX NAME)



RN 32531-68-3 CAPLUS
CN Benzenemethanamine, N-[2-[bis(4-methoxyphenyl)methyl]-1-azabicyclo[2.2.2]oct-3-ylidene]- (CA INDEX NAME)

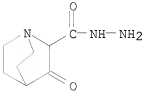




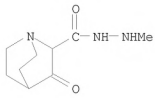
L15 ANSWER 116 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:487840 CAPLUS
DOCUMENT NUMBER: 73:87840
ORIGINAL REFERENCE NO.: 73:14357a,14360a
TITLE: Synthesis and properties of 3-hydroxypyrazolo[4,3-b]quinuclidine
AUTHOR(S): Mikhlina, E. E.; Vorob'eva, V. Ya.; Turchin, K. F.; Kostyuchenko, N. P.; Sheinker, Yu. N.; Yakhontov, L. N.
CORPORATE SOURCE: Vses. Nauch.-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1970), (5), 651-6
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The influence of the quinuclidine system on the third condensed ring was studied. The mixture of 3 g 2-carbethoxy-3-oxoquinuclidine (I), 12 ml EtOH, and 2 g N2H4 reacts at room temperature 3 hr, to form, 96% 3-oxoquinuclidine-2-carboxylic acid hydrazide (II), which decomps. to 72% 3-hydroxypyrazolo-[4,3-b]quinuclidine (III), m. 290.5°, when dissolved in boiling water. The yield increases to 98-9% after prolonged boiling or after heating in vacuo. III was also obtained directly from I and N2H4 at higher temps. III.HCl m. 208-10°; III.2HCl m. 199-200°; III.Ag salt m. 238° (decomposition). Methylation of III with Me2SO4 yielded its 2-Me derivative, m. 222-4°; hydrochloride m. 248-50°. Treatment of 1 mole III with 1 or 2 moles BzCl, resp., gives 61.3% 1-Bz derivative, m. 205-7°, or 84.5% 1-Bz derivative of the 3-benzoate of III, m. 148-50°. III reacts with acrylonitrile under reflux to form 36.8% 1-(β-cyanoethyl) derivative of III, m. 222-3.5°. Reaction of III with boiling Ac2O yields 56% 1-acetyl derivative of the 3-acetate of III, m. 127-8°; hydrochloride m. 214-17°; 1-acetyl derivative of III, m. 212-14°, was obtained by saponifying the 3-acetate or by treatment with Ac2O-pyridine mixture at room temperature Similarly to III, 44% methylhydrazide of 3-oxoquinuclidine-2-carboxylic acid (IV), m. 227-30°, was prepared from 3 g I and a solution of 2.44 g NaOH and 4.38 g methylhydrazine sulfate in 20 ml EtOH. IV heated gave 98% 1-Me derivative of III, m. 244°; dihydrochloride m. 194-7° (decomposition).

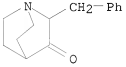
IT 28710-66-9P 28710-77-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28710-66-9 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, hydrazide (8CI) (CA INDEX NAME)



RN 28710-77-2 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, 2-methylhydrazide (8CI) (CA INDEX NAME)


O
N
C
NH
NHMe
O

L15 ANSWER 117 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:487765 CAPLUS
DOCUMENT NUMBER: 73:87765
ORIGINAL REFERENCE NO.: 73:14341a,14344a
TITLE: Preparation of 3,4,4a,5,11,11a-hexahydro-1,4-ethano-1H-benzo[5,6]cyclohepta[1,2-b]pyridin-6-(2H)one
AUTHOR(S): Villani, Frank J.; Wefer, Elizabeth A.
CORPORATE SOURCE: Dep. of Med. Chem., Schering Co., Bloomfield, NJ, USA
SOURCE: Journal of Heterocyclic Chemistry (1970), 7(4), 973-4
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 73:87765
GI For diagram(s), see printed CA Issue.
AB The title compound (I) is prepared by the cyclization of 2-benzyl-3-carboxymethylquinuclidine (II) with polyphosphoric acid or by the treatment of II acid chloride with AlCl3. 2-Benzylidene-3-quinuclidinone (III) is converted to the 2-benzyl derivative, which is treated with Et (diethylphosphono)acetate, and reduced to give II.
IT 28281-22-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28281-22-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(phenylmethyl)- (CA INDEX NAME)



L15 ANSWER 118 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:456081 CAPLUS
DOCUMENT NUMBER: 73:56081
ORIGINAL REFERENCE NO.: 73:9217a,9220a
TITLE: Analgesic 2,3-heterocyclic fused quinuclidines and 3-substituted quinuclidine-2-carboxylate derivatives
INVENTOR(S): Remers, William A.; Gibs, Gabriel J.; Weiss, Martin J.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3501471	A	19700317	US 1966-580894	19660921 <--
PRIORITY APPLN. INFO.:			US 1966-580894 A	19660921

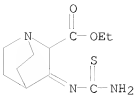
GI For diagram(s), see printed CA Issue.

AB The title compds. (I, where XYZ = pyrazolino, pyridazolino, pyrimidino, triazolino, or isoxazolino fusions) are central nervous system depressants and analgesic. Et 3-quinuclidinone-2-carboxylate-HCl (II) (7 g) and 25 ml N2H4.H2O was refluxed 16 hr and the product treated with 30 ml N HCl to yield pyrazol[3]ino[4,3-b]quinuclidin-3-one-HCl, m. 213-16°. Similarly, II and MeNHNH2 gave 2-methylpyrazol[3]ino[4,3-b]quinuclidin-3-one, m. 217-20° (CH2Cl2-n-C6H14). II (7 g), 2.9 g guanidine-HCl, and 60 ml EtOH was refluxed 2 hr to yield Et 2,3-didehydro-3-guanidinoquinuclidine-2-carboxylate-2HCl.H2O, m. 179-81°, which with EtONa in EtOH gave 2-amino-3H-pyrimidino[5,4-b]quinuclidin-4-one guanidinate hemihydrate, m. 258° (EtOH). II and thiourea was refluxed 24 hr in EtOH to yield Et 3-thiocarbamoyliminoquinuclidine-2-carboxylate-HCl.EtOH. 2,3-Didehydroquinuclidine-2,3-dicarboxylic acid was treated with AcCl and Ac2O to give the anhydride, which with anhydrous NH3 in THF gave 2,3-didehydroquinuclidine-2,3-dicarboxylic acid imide. 2,3-Didehydroquinuclidine, and PhN3 gave 1-phenyl-v-triazol[2]ino[4,5-b]-quinuclidine, m. 160-3°. Me 2,3-didehydroquinuclidine-3-carboxylate (III) (0.84 g), 1.6 g N-(α-chlorobenzylidene)-N'-phenylhydrazine, and 25 ml THF was treated with 0.81 g Et3N in 10 ml THF the product treated with HCl to give Me 2,7-diphenylpyrazol[5]ino[3,4-b]quinuclidine-6a-carboxylate-HCl, m. 223-35°. III and Ph3N gave Me 3-phenyl-v-triazol[1]ino[4,5-b]quinuclidine-7a-carboxylate, m. 143.5-5.5°.

IT 27952-10-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 27952-10-9 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-[(thiocarbamoyl)imino]-, ethyl ester, hydrochloride (8CI) (CA INDEX NAME)



● x HCl

L15 ANSWER 119 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:435237 CAPLUS
DOCUMENT NUMBER: 73:35237
ORIGINAL REFERENCE NO.: 73:5837a,5840a
TITLE: Analgesic 2,3-heterocyclic fused quinuclidines and 3-substituted quinuclidine-2-carboxylate derivatives
INVENTOR(S): Remers, William A.; Gibs, Gabriel J.; Weiss, Martin J.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3501471		19700317	US	19660921 <--

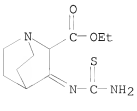
GI For diagram(s), see printed CA Issue.

AB Title compds., useful as central nervous system depressants and analgesic agents, were prepared Thus, 7 g Et 3-quinuclidinone-2-carboxylate-HCl hydrochloride (I) and 25 ml N2H4.H2O was refluxed 16 hr, to yield pyrazol[3]ino[4,3-b]quinuclidin-3-one-HCl, m. 213-16°. Similarly, I and MeNH-NH2 gave 2-methylpyrazol[3]ino[4,3-b]quinuclidin-3-one (II), m. 217-20° (CH2Cl2-n-C6H14). I (7 g), 2.9 g guanidine-HCl, and 60 ml EtOH was refluxed 2 hr to yield Et 2,3-dehydro-3-guanidinoquinuclidine-2-carboxylate-2HCl.H2O, m. 179-81°, which treated with EtONa in EtOH gave 2-amino-3H-pyrimidino[5,4-b]quinuclidin-4-one guanidinate-0.5H2O, m. 258° (EtOH). I and thiourea was refluxed 24 hr in EtOH to yield Et 3-thiocarbamoyliminoquinuclidine-2-carboxylate-HCl alcoholate, yellow glassy solid. 2,3-Dehydroquinuclidine-2,3-dicarboxylic acid was treated with AcCl and Ac2O to give the anhydride, oil, which was converted with anhydrous NH3 in THF into 2,3-dehydroquinuclidine-2,3-dicarboxylic acid imide, white solid. 2,3-Dehydroquinuclidine and PhN3 gave 1-phenyl-v-triazol[2]ino[4,5-b]quinuclidine, m. 160-3°. Me 2,3-dehydroquinuclidine-3-carboxylate (III) (0.84 g), 1.6 g N-(α-chlorobenzylidine)-N'-phenylhydrazine, and 25 ml THF was cooled in an ice bath, treated with 0.81 g Et3N in 10 ml THF, and the mixture kept 16 hr to give Me 2,7-diphenylpyrazol[5]ino-[3,4-b]quinuclidine-6a-carboxylate-HCl, m. 223-35°. III and Ph3N gave Me 3-phenyl-v-triazol[1]ino[4,5-b]quinuclidine-7a-carboxylate, m. 143.5-5.5°.

IT 27952-10-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 27952-10-9 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-[(thiocarbamoyl)imino]-, ethyl ester, hydrochloride (8CI) (CA INDEX NAME)



●x HCl

L15 ANSWER 120 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:403814 CAPLUS
DOCUMENT NUMBER: 73:3814
ORIGINAL REFERENCE NO.: 73:649a,652a
TITLE: 2-[4'-(Chloro)-benzydryl]-3-quinuclidinols as central nervous system stimulants
INVENTOR(S): Warawa, Edward J.; Mueller, Nancy Jean
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3506673	A	19700414	US 1968-717405	19680329 <--
PRIORITY APPLN. INFO.:			US 1968-717405 A	19680329

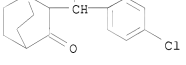
GI For diagram(s), see printed CA Issue.

AB A grignard reagent was prepared from 25.1 g PhBr in 200 ml anhydrous Et2O, 4.28 g Mg turnings and a trace of iodine; after refluxing 2.5 hr and cooling (ice bath), a solution of 26.52 g 2-(4-chlorobenzylidenyl-3-quinuclidinone in 400 ml C6H6 was added dropwise over 3.75 hr, and the mixture stirred overnight at room temperature crystallized from alc. to give 44.8% 2-(4-chlorobenzhydryl)-3-quinuclidinone (I) m. 145-80°. A soln of 1 g I, 3.5 g (iso-PrO)3Al, and 20 ml anhydrous iso-PrOH was heated on a steam bath while N was slowly passed in 2.5 hr, then worked up to give the corresponding alc., (50:50 mixture of the cis isomers containing a trace of trans isomer) separated by chromatog. to give 330 mg α-cis isomer, m. 169-70.5° (MeOH); 250 mg mixt of α-and β-isomers; and 350 mg β-cis isomer, m. 236-6.5° (decomposition) (MeOH).

IT 27655-54-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 27655-54-5 CAPLUS

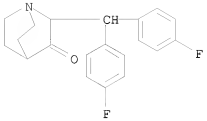
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[(4-chlorophenyl)phenylmethyl]- (CA INDEX NAME)



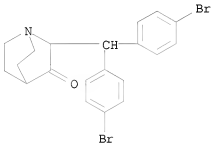
L15 ANSWER 121 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:31644 CAPLUS
DOCUMENT NUMBER: 72:31644
ORIGINAL REFERENCE NO.: 72:5785a,5788a
TITLE: 2-(4,4'-Difluoro- and 2-(4,4'-dibromobenzhydryl)-3-quinuclidinol
INVENTOR(S): Warawa, Edward J.; Mueller, Nancy Jean
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: Ger. Offen., 31 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1915142	A	19691002	DE 1969-1915142	19690325 <--
US 3506672	A	19700414	US 1968-717389	19680329 <--
NL 6904655	A	19691001	NL 1969-4655	19690326 <--
GB 1257387	A	19711215	GB 1969-1257387	19690326 <--
DK 122128	B	19720124	DK 1969-1657	19690326 <--
BE 730701	A	19690929	BE 1969-730701	19690328 <--
FR 2005129	A5	19691205	FR 1969-9467	19690328 <--
CH 499520	A	19701130	CH 1969-499520	19690328 <--

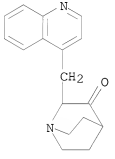
PRIORITY APPLN. INFO.: US 1968-717389 A 19680329
GI For diagram(s), see printed CA Issue.
AB The title products (I), for the treatment of arthritis, rheumatism, and other inflammations, are prepared by reacting 3-quinuclidone (II) with p-fluorobenzaldehyde (III) or p-bromobenzaldehyde to give 2-(4-fluoro)benzylidene-3-quinuclidone (IV) or the Br analog, which is treated with p-BrC6H4F or p-Br2C6H4 in a Grignard reaction to give 2-(4,4'-difluorobenzhydryl)-3-quinuclidone (V), which is reduced with Al isopropoxide to give (±)-cis-I (X = F) or with NaBH4 to give a mixture of cis- and tr ans-I, which is repeatedly oxidized with Ph2CO and again reduced with NaBH4 until pure trans-I is obtained. Thus, 12.5 g. II, 12.4 g III, and 1 pellet NaOH in 25 ml EtOH was refluxed 2.5 hr to give 20.9 g. IV, m. 118.5-20.5°. To 175 g p-BrC6H4F, 26.7 g Mg, and a trace of iodine in 900 ml Et2O was added 151 g IV in 19 l. benzene in 6.5 hr to give 143.1 g V, m. 160-2.5°. V (120 g) and 200 g Al isopropoxide in iso-PrOH gave 98.16 g (±)-cis-I (X = F), m. 197-8° (MeOH), HCl salt m. 297-300°. Salts were prepared with (-)-mandelic acid and with (±)-mandelic acid; the optically active mandelates m. 228-30°; from these were made (+)-cis-I, m . 185-6°, [α]25D 20° and its antipode, [α]25D -20°, m. 185-6°. The optically active HCl salts have [α]25D 27° and -27°. IV (5 g) in 175 ml EtOH and 25 ml CH2Cl2 was treated with 1.16 g. NaBH4 to give 5.31 g mixture of (±)-cis- and trans-I. This was treated in 45 ml benzene with 11.56 g Ph2CO and 1.42 g KH in 35 ml benzene and refluxed 0.75 hr to give 4.69 g mixed trans-I (X = F) and IV, which was reduced with NaBH4 as above. The whole process was repeated twice to obtain 0.85 g (±)-trans-I, m. 190-2°. Similarly was obtained 84.5% 2-(4-bromo)benzylidene-3-quinuclidone, m. 125-6°, and from this 32% 2-(4,4'-dibromobenzhydryl)-3-quinuclidone, m. 191-3°; this gave on reduction with Al isopropoxide 68.3% (±)-cis-I (X = Br), m. 205-6°.
IT 24802-69-5P 24802-70-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24802-69-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[bis(4-fluorophenyl)methyl]- (CA INDEX NAME)



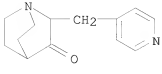
RN 24802-70-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[bis(4-bromophenyl)methyl]- (CA INDEX NAME)



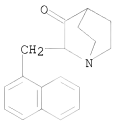
L15 ANSWER 122 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:491727 CAPLUS
DOCUMENT NUMBER: 71:91727
ORIGINAL REFERENCE NO.: 71:17095a,17098a
TITLE: Mass spectrometric fragmentation in the Cinchona alkaloid series
AUTHOR(S): Begue, Jean P.; Fetizon, Marcel
CORPORATE SOURCE: Lab. Stereochim., Fac. Sci., Orsay, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1969), (4), 1251-4
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB Major cleavage of quinine in mass spectrometry yields fragments in which H is transferred from quinuclidine to quinoline moieties. In expts. with I-2-d and II-2- and -3-d, the 2-H (D) was transferred to the aryl fragment during mass spectral cleavage. Condensing aromatic aldehydes and 3-quinuclidone with NaOEt in EtOH gave III (R, m.p., and % yield listed): 4-quinolyl, 154-5°, 60; Ph, 133°, 85; 4-pyridyl, 140°, 46; 1-naphthyl, 149°, 75. Hydrogenation of III over Pd gave I (R, m.p., and % yield listed): 4-quinolyl, 126-7°, 55; Ph, 84-5°, 67; 4-pyridyl, 114-16°, 70; 1-naphthyl, 97-8°, 72. I with NaBH4 yielded II (R, m.p., and % yield listed): 4-quinolyl, 215°, 52; (prepared by hydrogenation over Pt), 156-7°, -; 4-pyridyl, 129-30°, 60; 1-naphthyl, 169.5-70° and 211-13.5° (stereoisomers), -. I with D2O and K2CO3 gave I-2-d, which were reduced with LiAlH4 to II-2-d. I with LiAlD4 gave II-3-d.
IT 24177-70-6P 24177-72-8P 24177-73-9P
24177-77-3P 24177-78-4P 24177-79-5P
24177-80-8P 28281-22-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24177-70-6 CAPLUS
CN 11-Norcinchonan-7-one, (8ξ)- (9CI) (CA INDEX NAME)



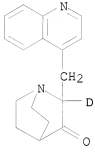
RN 24177-72-8 CAPLUS
CN 3-Quinuclidinone, 2-(4-pyridylmethyl)- (8CI) (CA INDEX NAME)



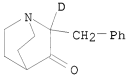
RN 24177-73-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(1-naphthalenylmethyl)- (CA INDEX NAME)



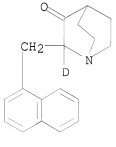
RN 24177-77-3 CAPLUS
CN 3-Quinuclidinone-2-d, 2-(4-quinolylmethyl)- (8CI) (CA INDEX NAME)



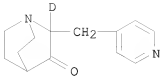
RN 24177-78-4 CAPLUS
CN 3-Quinuclidinone-2-d, 2-benzyl- (8CI) (CA INDEX NAME)



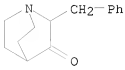
RN 24177-79-5 CAPLUS
CN 3-Quinuclidinone-2-d, 2-(1-naphthylmethyl)- (8CI) (CA INDEX NAME)



RN 24177-80-8 CAPLUS
CN 3-Quinuclidinone-2-d, 2-(4-pyridylmethyl)- (8CI) (CA INDEX NAME)



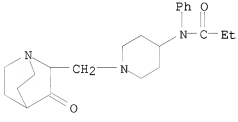
RN 28281-22-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(phenylmethyl)- (CA INDEX NAME)



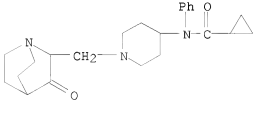
L15 ANSWER 123 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:491343 CAPLUS
DOCUMENT NUMBER: 71:91343
ORIGINAL REFERENCE NO.: 71:17003a,17006a
TITLE: 2-(4-Anilinopiperidinomethyl)-3-quinuclidinones exhibiting antidepressant activity
INVENTOR(S): Biel, John H.; Hopps, Harvey B.
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3462442	A	19690819	US 1965-515183	19651220 <--
PRIORITY APPLN. INFO.:			US 1965-515183 A	19651220

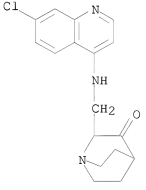
GI For diagram(s), see printed CA Issue.
AB Title compds. with the described activity are prepared Thus, 50 g. 3-quinuclidinone, 50 g. 37% aqueous HCHO, and 68 g. 40% aqueous Me2NH in 70 ml. absolute EtOH is refluxed 22 hrs. to give 43 g. 2-methylene-3-quinuclidinone (I), b10 90-110°. A solution of 5.48 g. I and 9.28 g. 4-(N-propionylanilino)piperidine in 100 ml. MeOH is kept 24 hrs. to give II, m. 123-4°. Similarly prepared is III, m. 129-31°.
IT 23851-86-7P 23851-87-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23851-86-7 CAPLUS
CN Propionanilide, N-[1-[(3-oxo-2-quinuclidinyl)methyl]-4-piperidyl]- (8CI) (CA INDEX NAME)



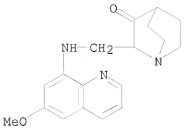
RN 23851-87-8 CAPLUS
CN Cyclopropanecarboxanilide, N-[1-[(3-oxo-2-quinuclidinyl)methyl]-4-piperidyl]- (8CI) (CA INDEX NAME)



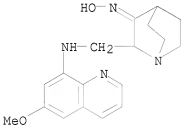
L15 ANSWER 124 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:430341 CAPLUS
DOCUMENT NUMBER: 71:30341
ORIGINAL REFERENCE NO.: 71:5589a,5592a
TITLE: Antimalarials. Some quinuclidine derivatives of 7-chloro-4-aminoquinoline and 6-methoxy-8-aminoquinoline
AUTHOR(S): Singh, Tara; Stein, Robert G.; Koelling, Harlan H.; Hoops, John F.; Biel, John H.
CORPORATE SOURCE: Res. Lab., Aldrich Chem. Co., Inc., Milwaukee, WI, USA
SOURCE: Journal of Medicinal Chemistry (1969), 12, 524-6
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Thirteen quinoline compds. containing quinuclidine rings in side chains were prepared and tested for their antimalarial activity against Plasmodium berghei in mice. 7-Chloro-4-(3-oxoquinuclidinyl-2-methyleneamino)quinoline (I) and 7-chloro-4-(3-hydroxyquinuclidinyl-2-methyleneamino)quinoline (II) were curative; I cured 2 mice at 160 mg./kg. and all 5 in the test at 640 mg./kg., while II showed slight activity at 160 and 320 mg./kg. and cured all 5 mice at 640 mg./kg. All other compds. were inactive and toxic.
IT 21566-68-7P 22776-50-7P 22776-52-9P
22950-03-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21566-68-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-[[(7-chloro-4-quinolinyl)amino]methyl]- (CA INDEX NAME)



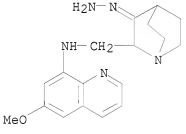
RN 22776-50-7 CAPLUS
CN 3-Quinuclidinone, 2-[[(6-methoxy-8-quinolyl)amino]methyl]- (8CI) (CA INDEX NAME)



RN 22776-52-9 CAPLUS
CN 3-Quinuclidinone, 2-[[(6-methoxy-8-quinolyl)amino]methyl]-, oxime (8CI)
(CA INDEX NAME)



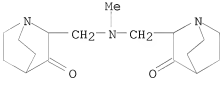
RN 22950-03-4 CAPLUS
CN 3-Quinuclidinone, 2-[[(6-methoxy-8-quinolyl)amino]methyl]-, hydrazone
(8CI) (CA INDEX NAME)



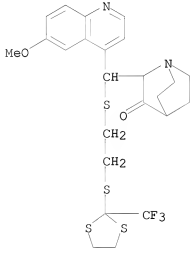
L15 ANSWER 125 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:459119 CAPLUS
DOCUMENT NUMBER: 69:59119
ORIGINAL REFERENCE NO.: 69:11047a,11050a
TITLE: 2-Methylene-3-quinuclidinone
INVENTOR(S): Biel, John H.; Hopps, Harvey B.; Bader, Henryk
PATENT ASSIGNEE(S): Aldrich Chemical Co., Inc.
SOURCE: U.S., 2 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3384641	A	19680521	US 1967-668941	19670919 <--
PRIORITY APPLN. INFO.:			US 1967-668941 A	19670919

GI For diagram(s), see printed CA Issue.
AB The title compound (I) is prepared by heating the Mannich reaction product of 3-quinuclidinone (II), Me2NH, and HCHO; it is used to sep. tertiary from primary and secondary amines. Thus, 200 g. II, 270 g. 40% Me2NH, 194.8 g. 37% HCHO, 250 ml. EtOH, and 100 ml. water was refluxed 1 hr., held 17 hrs. at 70°, and worked up to give 203 g. I, b7 91-2°, n2D0 1.5110; HCl salt m. 284-8°. A mixture of pyridine and piperidine was separated by distillation in the presence of I. The piperidine distilled only after its reaction product with I decomposed MeNH2 was also purified by adding 13.7 g. I in 20 ml. MeOH to 3.88 g. 40% aqueous MeNH2 and heating 1 hr. at 50° to give 11 g. 2,α'-methyliminobis(2-methyl-3-quinuclidinone) monohydrate, m. 90-2°, which was decomposed by gentle heating to pure MeNH2, leaving I as a residue.
IT 19576-25-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19576-25-1 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2,2'-[(methylimino)bis(methylene)]bis- (9CI) (CA INDEX NAME)



L15 ANSWER 126 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:427579 CAPLUS
DOCUMENT NUMBER: 69:27579
ORIGINAL REFERENCE NO.: 69:5155a,5158a
TITLE: Synthetic quinine analogs. I. Synthesis and some chemical transformations of 6'-methoxy-7-oxo-8-rubene
AUTHOR(S): Bender, D. R.; Coffen, D. L.
CORPORATE SOURCE: Univ. of Colorado, Boulder, CO, USA
SOURCE: Journal of Organic Chemistry (1968), 33(6), 2504-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB NaOEt-catalyzed condensation of 6-methoxyquinoline-4-carboxaldehyde with 3-quinuclidinone produces 6'-methoxy-7-oxo-8-rubene (I) in high yield. Of the 2 possible geometrical isomers, only that with the ketone function trans to the quinoline ring is formed. Reduction of I affords an allylic alc. whose p-nitrobenzoate is completely isomerized to the opposite geometrical isomer in refluxing HOAc. I is not ketalized by 1,2-ethanedithiol in refluxing F3CCO2H involving 1 mol. of ketone, 2 of 1,2-ethanedithiol, and 1 of F3CCO2H. A by-product of the reaction results from the condensation of 3 mols. of 1,2-ethanedithiol with 2 of F3CCO2H. Pyrazoline derivs. of I resulting from 1,3-dipolar addition of CH2N2 and condensation with hydrazine are described. 24 references.
IT 16526-37-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16526-37-7 CAPLUS
CN Orthoacetic acid, trifluorotrithio-, cyclic ethylene ester, ester with 2-[[(2-mercaptoethyl)thio](6-methoxy-4-quinolyl)methyl]-3-quinuclidinone, (±)- (8CI) (CA INDEX NAME)

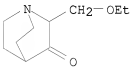


L15 ANSWER 127 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:84473 CAPLUS
DOCUMENT NUMBER: 64:84473
ORIGINAL REFERENCE NO.: 64:15837a-b
TITLE: Systems with bridgehead nitrogen. β-Ketols of the 1-azabicyclo[2.2.2]octane series
AUTHOR(S): Nielsen, Arnold T.
CORPORATE SOURCE: Chem. Div., U.S. Naval Ordnance Test Sta., China Lake, CA
SOURCE: Journal of Organic Chemistry (1966), 31(4), 1053-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

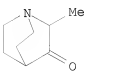
AB The prepns. and chemical behavior of the β-ketols incorporating the 1-azabicyclo [2.2.2] octane ring are described. Three different structural types are represented in this study. Methylolation of 3-quinuclidinone with excess formaldehyde (potassium carbonate catalyst under appropriate conditions) led to 2,2-bismethylol-3-quinuclidinone (I) or 2-methylene-3-quinuclidinone (II). 2-Methylol-3-quinuclidinone (III) was prepared by hydration of II cation. Starting with 4-acetylpiperidine and its N-benzyl derivative, syntheses of 4-hydroxymethyl-3-quinuclidinone (IV) and 4-acetyl-3-quinuclidinol (V) were achieved. The bridgehead IV was extremely stable whereas V underwent facile retrograde aldolization in basic media. I readily loses one methylol group in base leading to III, which dehydrates with extreme ease rather than undergo demethylolation.

IT 5291-13-4P, 3-Quinuclidinone, 2-(ethoxymethyl)- 5291-14-5P, 3-Quinuclidinone, 2-methyl- 5291-27-0P, 3-Quinuclidinone, 2-(hydroxymethyl)- 5291-32-7P, 3-Quinuclidinone, 2-(hydroxymethyl)-2-(methoxymethyl)- 5291-33-8P, 3-Quinuclidinone, 2-(ethoxymethyl)-, picrate 5291-34-9P, 3-Quinuclidinone, 2-methyl-, picrate 5291-35-0P, 3-Quinuclidinone, 2-(hydroxymethyl)-, hydrochloride
RL: PREP (Preparation)
(preparation of)

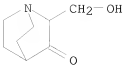
RN 5291-13-4 CAPLUS
CN 3-Quinuclidinone, 2-(ethoxymethyl)- (7CI, 8CI) (CA INDEX NAME)



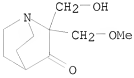
RN 5291-14-5 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-methyl- (CA INDEX NAME)



RN 5291-27-0 CAPLUS
CN 3-Quinuclidinone, 2-(hydroxymethyl)- (7CI, 8CI) (CA INDEX NAME)



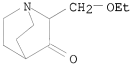
RN 5291-32-7 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(hydroxymethyl)-2-(methoxymethyl)- (CA INDEX NAME)



RN 5291-33-8 CAPLUS
CN 1-Azabicyclo[2.2.2]octan-3-one, 2-(ethoxymethyl)-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

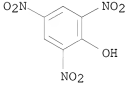
CM 1

CRN 5291-13-4
CMF C10 H17 N O2



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



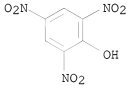
RN 5291-34-9 CAPLUS
CN 3-Quinuclidinone, 2-methyl-, picrate (7CI, 8CI) (CA INDEX NAME)

CM 1

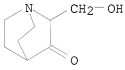
CRN 5291-14-5
CMF C8 H13 N O

CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



RN 5291-35-0 CAPLUS
CN 3-Quinuclidinone, 2-(hydroxymethyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



● HCl

L15 ANSWER 128 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:9663 CAPLUS
DOCUMENT NUMBER: 60:9663
ORIGINAL REFERENCE NO.: 60:1697e-h,1698a-h,1699a
TITLE: Quinuclidine series. VII. Solvolysis of 2-(α-chlorobenzyl)quinuclidine. The heterocinchonine rearrangement
AUTHOR(S): Braschler, V.; Grob, C. A.; Kaiser, A.
CORPORATE SOURCE: Univ. Basel, Switz.
SOURCE: Helvetica Chimica Acta (1963), 46(7), 2646-58
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 60:9663

AB cf. CA 53, 4278e. The rate and the products of the hydrolysis of 2-(α-chlorobenzyl)quinuclidine (I) do not provide evidence for the participation of the quinuclidine N in the ionization step, and no product derived from a heterocinchonine rearrangement could be isolated. 2-Benzyl-2-dehydroquinuclidine (II) and 2-benzylidenequinuclidine (III) possess abnormal spectral and chemical properties ascribable to steric inhibition of the vinylamine-type mesomerism. Et isonicotinate (151 g.) and 167 g. BrCH2CO2Et in 500 cc. EtOH kept at room temperature overnight, refluxed 4 hrs., hydrogenated 0.5-1 hr. at 90°/100 atmospheric over 15 g. 10% Pd-C, filtered, the filtrate evaporated at 50-60°, the semicryst. residue treated with cooling and shaking with 500 cc. cold H2O, 500 cc. CHCl3, and 150 g. K2CO3 in 250 cc. H2O, and the organic layer worked up yielded 180-90° 4-carbethoxy-1-carbethoxymethylpiperidine (IV), b0.2 111-13°, n20D 1.4585, d1515 1.057. IV (100 g.) in 250 cc. absolute MePh added dropwise during 1.5 hrs. to KOEt (from 39.096 g. K and 60 cc. EtOH in 162 cc. dry MePh) the mixture stirred 4 hrs. at 130°, cooled, the MePh decanted, extracted with 50 cc. H2O, the residue dissolved in 300 cc. EtOH, combined with the aqueous extract, the solution adjusted with 100 cc. 10N HCl with cooling and stirring to pH 7 below 30°, cooled to 0°, filtered, the filtrate adjusted with about 2 cc. AcOH to pH 4, concentrated to about 200 cc., treated with 20 cc. saturated aqueous KHCO3, and extracted with CHCl3 yielded 57 g. 2-carbethoxy-3-quinuclidone (V), b0.02 98-103°, m. 116-20° (absolute EtOH-Et2O). V (20 g.), 80 cc. dry Et3N, and 100 cc. absolute EtOH hydrogenated over about 5 g. Raney Ni under ambient conditions yielded 10.9 g. 2-carbethoxy-3-hydroxyquinuclidine (VI) isomer A (VII), m. 147-8° (Me2CO), (sublimation); the filtrate was evaporated and the cryst, residue (9 g.) chromatographed on 200 g. Al2O3 to give 2.34 g. VII, 4.7 g. isomer mixture, m. 72-105°, and 1.98 g. VI isomer B, m. 100-2°; VI.MeI, m. 175-8° (decomposition) (EtOH-Et2O). VI (21.1 g.) and 150 cc. Ac2O refluxed 6 hrs., the mixture evaporated, the oily residue partitioned between 200 cc. Et2O and 50 cc. 2N HCl, the Et2O phase extracted with 2N HCl, the combined aqueous solns. saturated with solid K2CO3, and extracted with Et2O gave 14.4 g. 2-carbethoxy-2-dehydroquinuclidine (VIII), b12 128-30°, n25D 1.4955, and 1.1 g. acetate of VI, b12 130-63°. VIII (12.7 g.) in 65 cc. EtOH hydrogenated 1 hr. over 600 mg. 10% Pd-C under ambient conditions yielded 12.1 g. 2-carbethoxyquinuclidine, b11 119-20°, n25D 1.4752, b11 119-20°; picrate m. 120° (EtOH). VIII (10 g.) and 150 cc. saturated NH3-MeOH heated 15 hrs. at 100° in an autocalve gave 7.5 g. 2-CONH2 analog (IX) of VIII, m. 178-81° (Me2CO). IX (5.45 g.) in 50 cc. MeOH and 25 cc. H2O hydrogenated 2 hrs. over Raney Ni W-7 under ambient conditions yielded 4.9 g. 2-carbamoylquinuclidine (X), m. 148-9°(Me2CO). 2-Carbethoxyquinuclidine (1.2 g.) and 10 cc. NH3-MeOH (saturated at 20°) heated 48 hrs. at 100° in a sealed

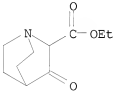
tube gave 0.81 g. X, m. 145-6° (Me2CO). IX (5.6 g.) in 45 cc. Et3N and 25 cc. CHCl3 mixed with 10.5 g. P2O5 g. and 50 g. sand, refluxed 30 hrs., cooled, the supernate decanted, the residual oil washed with Et2O, the residue treated with saturated aqueous K2CO3 and extracted with Et2O, and the combined washings, and decantate worked up yielded 0.92 g. unreacted IX, m. 177-80°; the mother liquor distilled gave 2 g. 2-CN analog of VIII, b11 120-3°, n 24.5D 1.5068. X (12.2 g.), 22.5 g. P2O5, and 50 g. sand refluxed 26 hrs. with 90 cc. dry Et3N and 60 cc. dry CHCl3 and similarly worked up yielded 8.25 g. 2-cyanoquinuclidine (XI), b13 105-21°; picrate m. 216-26° (decomposition) (Me2CO-EtOH); XI.MeI m. 247-50° (decomposition) (absolute EtOH). X (9.4 g.), 50 cc. Ac2O, and 50 cc. Et3N refluxed 10 hrs. yielded 4 g. XI, b13 105-21°. XI (17.4 g.) in 300 cc. dry C6H6 added dropwise during 1 hr. to PhMgBr from 6.5 g. Mg, 40.2 g. PhBr, and 170 cc. dry Et2O and the mixture refluxed 4 hrs. yielded 20.9 g. 2-benzoylquinuclidine (XII), m. 88-9.5° (Et2O); the residue from the mother liquor sublimed at 120-40°/11 mm. gave 1.35 g. XII, m. 86-9°; picrate m. 174-8° (EtOH); methiodide m. 196-8° (Me2CO). XII (1 g.) and 0.335 g. NH2OH.HCl in 20 cc. MeOH refluxed 24 hrs. yielded the oxime of XII, m. 194-5.5° with sublimation (AcOEt); picrate m. 194-8° with sublimation (EtOH) XII (4.0 g.) in 50 cc. dry Et2O added dropwise during 10 min. with stirring to 0.5 g. LiAlH4 in 50 cc. dry Et2O, the mixture refluxed 3 hrs., stirred 12 hrs. at room temperature, and decomposed with 30 cc. iced H2O and 25 cc. concentrated HCl yielded the mixed isomeric 2-(α-hydroxybenzyl)quinuclidine (XIII), which-recrystd. repeatedly from Me2CO gave 800 mg. isomer A (XIIIa), m. 142-4° [picrate m. 191-4° (EtOH)]; the residue (2.9 g.) from the mother liquor chromatographed on 60 g. Al2O3 gave the isomer B (XIIIb), m. 75-6.5° (petr. ether) [picrate m. 183-6° (EtOH)]. XIII (3 g.) and 30 cc. SOCl2 refluxed 12 hrs., the mixture evaporated, and the residue evaporated twice with C6H6 and fractionally recrystd. from absolute EtOH yielded I.HCl isomer A (Ia.HCl), m. 238-40° (absolute EtOH-Et2O) [picrate m. 183-6° (EtOH)], and I.HCl isomer B (Ib.HCl), m. 245-9.5° (decomposition) [picrate m. 173-4° (EtOH)]. Ia (1.89 g.) in 5 cc. absolute EtOH refluxed 3 hrs. with 3.5 g. KOH in 20 cc. absolute EtOH yielded 1.39 g. III isomer A (IIIa), b12 168-70° [picrate m. 149-50° and then 167-9° (EtOH)]. Ib (500 mg.) and 1 g. KOH in 10 cc. absolute EtOH refluxed 14 hrs. yielded 394 mg. oily III isomer B (IIIb) [picrate m. 162-3° and then 180-1° (iso-PrOH-Me2CO)]. Quinuclidone-HCl (8.5 g.) and 15 g. BzH refluxed 10 hrs. with 7.5 g. KOH in 150 cc. absolute EtOH yielded 8.07 g. 2-benzylidene-3-quinuclidone (XIV), m. 134-7° (MeOH) [picrate m. 180-4° (EtOH)]. XIV (11.05 g.) in 300 cc. MeOH hydrogenated under ambient conditions over Raney Ni, and the product fractionally recrystd. from Me2COMeOH yielded 7.7 g. 2-benzyl-3-hydroxyquinuclidine isomer A (XVa), m. 157-8° [picrate m. 128-32° (iso-PrOH); HCl salt m. 203-7° (MeOH-Me2CO-Et2O)]; the residue (2.85 g.) from the mother liquor chromatographed on 60 g. Al2O3 yielded 1.5 g. XV isomer B (XVb), m. 129-33° (Me2CO) [picrate, m. 159-62° (iso-PrOH)], and 1.3 g. mixed XVa and XVb. XVa (5 g.) and 50 cc. SOCl2 refluxed 70 hrs. gave 2 g. II, b0.005 62°, n23D 1.5485, which solidified at -15° [picrate m. 200-5° (Me2CO)], and 1.9 g. 2-benzyl-3-chloroquinuclidine, b0.005 73-5°, picrate m. 184-7° with a change to plates and then m. 201-3° (iso-PrOH). I.HCl (500 mg.) in 25 cc. EtOH hydrogenated about 2 hrs. over 50 mg. 10% Pd-C yielded 2-benzylquinuclidine-HCl (XVI.HCl), m. 268-9° (EtOH-Et2O) (with sublimation); picrate m. 184-6° (EtOH). IIIa or IIIb (200 mg.) in EtOH hydrogenated over Pd-C yielded XVI isolated as picrate, m. 183-6° (EtOH); XVI.HCl m. 270-2° (EtOH-Et2O). II (260 mg.) in 5 cc. EtOH hydrogenated over Raney Ni yielded XVI isolated as the picrate, m. 180.5-3.5° (iso-PrOH). I.HCl (2.0017 g.), 8 cc. N NaOH, 32.4 cc. H2O, and 32.4 cc. Me2CO heated 24 hrs. at 68°,

cooled, acidified with 2N HCl, concentrated to 20 cc. at 45°, basified with saturated aqueous K2CO3, and extracted with CHCl3, and the residue from the extract chromatographed on Al2O3 yielded 100 mg. substance which gave the picrate of IIIa, m. 145-50° and then 167-9° (EtOH), 110 mg. oil which yielded the picrate of XIII, m. 278-81° (EtOH) [free base m. 72-8° (petr. ether)], and 110 mg. oily C13H17NO (XVII); picrate m. 186-8° (EtOH); HCl salt m. 157-8° (decomposition) (iso-PrOH-Et2O). I.HCl (4 g.), 5.94 g. Et3N, 40 cc. H2O, and 40 cc. Me2CO refluxed 42 hrs., cooled, acidified with 2N HCl, concentrated to 30 cc., basified with saturated aqueous K2CO3, and extracted with Et2O, and the oily residue (3.1 g.) from the extract chromatographed on Al2O3 gave 103 mg. III, 210 mg. XIII, and 56 mg. XVII. I.HCl (1.3 g.) treated in the usual manner with K2CO3, the free base stirred 24 hrs. at room temperature in 100 cc. 60% aqueous Me2CO with 2 equivs. Ag2O, refluxed 24 hrs., filtered through Celite, acidified with 2N HCl, concentrated to 20 cc., basified with saturated aqueous K2CO3, and extracted with CHCl3, and the oily residue from the extract distilled gave 510 mg. yellow oil, b0.01 90-110°, which chromatographed on Al2O3 yielded 147 mg. III, 89 mg. XIII, and 155 mg. oily XVII.

IT 34286-16-3P, 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester
RL: PREP (Preparation)
(preparation of)

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



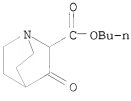
L15 ANSWER 129 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:410798 CAPLUS
DOCUMENT NUMBER: 57:10798
ORIGINAL REFERENCE NO.: 57:2192e-i
TITLE: Synthesis of 2,3-quinuclidinedicarboxylic acid
AUTHOR(S): Mikhlina, E. E.; Rubtsov, M. V.; Vorob'eva, V. Ya.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem.-Pharm. Res. Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1961), 31, 3251-5
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:10798

AB cf. CA 54, 9945i. Azeotropic removal of H2O from 69.3 g. KOH, 11. BuOH, and 100 ml. MePh, evaporation of the residue, and treatment with 120 g. 1-carbethoxymethyl-4-carbethoxypiperidine 5 hr. in MePh gave a viscous mass containing K salt of the enol of Bu 3-oxoquinuclidine-2-carboxylate, which treated with 10% AcOH followed by K2CO3 gave 43.5% Bu 3-oxo-quinuclidine-2-carboxylate, b0.6 137° m. 88°; HCl salt m. 163°. The latter treated with aqueous KCN at 5° gave 68.5% cyanohydrin, m. 107°. Similarly was prepared the cyanohydrin of the Et ester, m. 124-5°. This refluxed 25 hrs. with AcOH-HCl then esterified with EtOH-HCl gave some 3-quinuclidone, separated by sublimation, and 30% di-Et 3-hydroxyquinuclidine-2,3-dicarboxylate (I), b1.2 142°, m. 104-5°, also formed from the corresponding Bu ester cyanohydrin. Refluxing the di-Et ester with 1:1 HCl 5 hrs. gave 65% 3-hydroxyquinuclidine-2,3-dicarboxylic acid-HCl, decomposed at 126°. I with SOCl2 30 hrs. followed by aqueous K2CO3 gave 74.5% di-Et Δ2-dehydroquinuclidine-2,3-dicarboxylate, b0.5 130°; HCl salt m. 148.5°. This refluxed 5 hrs. with 1:1 HCl gave 99% Δ2-dehydroquinuclidine-2,3-dicarboxylic acid, decomposed at 240°; HCl salt, hygroscopic crystals, hydrolyzed by H2O. Hydrogenation over Pt gave quinuclidine-2,3-dicarboxylic acid-HCl, decomposed at 138°, which refluxed 5 hrs. with EtOH-HCl gave the di-Et ester (II), b0.4 115°, which with LiAlH4 gave 58% 2,3-bis(hydroxymethyl)quinuclidine, b0.3 150°; HCl salt, hygroscopic crystals. This and AcCl in refluxing CHCl3 5 hrs. gave 70% diacetate, b0.6 138-40°. II kept 7 days in H2O gave 83.5% 3-carbethoxyquinuclidine-2-carboxylic acid, decomposed at 188-9°.

IT 91554-81-3P, 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester, hydrochloride 91554-82-4P, 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester
RL: PREP (Preparation)
(preparation of)

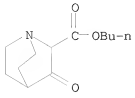
RN 91554-81-3 CAPLUS

CN 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 91554-82-4 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, butyl ester (7CI) (CA INDEX NAME)

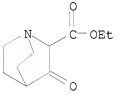


L15 ANSWER 130 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:50470 CAPLUS
DOCUMENT NUMBER: 54:50470
ORIGINAL REFERENCE NO.: 54:9945i,9946a-c
TITLE: Amino acids of the quinuclidine series
AUTHOR(S): Yakhontov, L. N.; Rubtsov, M. V.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Research Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 2343-8
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:50470

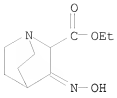
AB Keeping 1.1 g. 2-formylquinuclidine and 0.9 g. EtO2CCH2CN in 3 ml. pyridine with 5 drops piperidine 10 days gave a precipitate of 97.2% Et β-(2-quinuclidyl)-α-cyano-acrylate, m. 139.5-41° (picrate, m. 130.5-10°), which hydrogenated over Pt to α-aminomethyl-β-(2-quinuclidyl)propionic acid, isolated as dipicrate, decomposing 125°; the acid was isolated after the original reaction mixture was hydrogenated and then refluxed with concentrated HCl. Keeping an aqueous solution of Na salt of enol form of Et β-(2-quinuclidyl)-β-oxopropionate 1 day gave Na β-(2-quinuclidyl)-β-oxopropionate, decomposing 240°; this with HONH2 gave 93% β-(2-quinuclidyl)-β-oxopropionic acid oxime, an oil; di-HCl salt, decompose 284°; picrate, m. 167-70°. Hydrogenation of the oxime over Pt gave 78% β-(2-quinuclidyl)-β-aminopropionic acid isolated as di-HCl salt, decomposing 283°. To KOEt in dry MePh was added at 120° 1-carbethoxymethylisonipecotinic acid, the whole was refluxed 5 hrs., cooled, the precipitated K salt of Et 3-oxo-2-quinuclidinecarboxylate was separated and treated with dilute AcOH, yielding 75%
Et 3-oxo-2-quinuclidinecarboxylate, m. 109-10°. This with HONH2.HCl in EtOH gave 80% corresponding oxime, isolated as HCl salt, decomposing 196°. This, hydrogenated over Pt to 99.4% Et 3-amino-2-quinuclidinecarboxylate di-HCl salt, decomposing 185°. This heated with concentrated HCl 6 hrs. gave 91% 3-amino 2-quinuclidinecarboxylic acid di-HCl salt, decomposing 242°.

IT 34286-16-3 110056-51-4 117342-57-1
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 34286-16-3 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

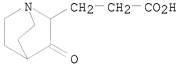


RN 110056-51-4 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester, oxime, hydrochloride (6CI) (CA INDEX NAME)

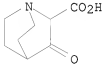


● HCl

RN 117342-57-1 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



IT 857019-15-9, 2-Quinuclidinecarboxylic acid, 3-oxo-
(derivs.)
RN 857019-15-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo- (CA INDEX NAME)



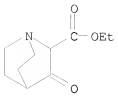
L15 ANSWER 131 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:50469 CAPLUS
DOCUMENT NUMBER: 54:50469
ORIGINAL REFERENCE NO.: 54:9945d-i
TITLE: Phenanthryl substituted barbiturates
AUTHOR(S): Giannini, M.; Fedi, M.; Russo, F.
CORPORATE SOURCE: Lab. chim. farm. A. Menarini, Florence
SOURCE: Bollettino Chimico Farmaceutico (1959), 98, 714-21
CODEN: BCFAAI; ISSN: 0006-6648
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Refluxing 2.26 g. 9-(chloromethyl)phenanthrene (I) with 62 ml. PrOH, adding 1.42 g. 5-methylbarbituric acid and 0.8 g. HCO2Na in 7 ml. H2O, refluxing 7 hrs., distilling the PrOH to a small volume, mixing the residue with 100 ml. H2O, filtering, and washing with C6H6 until the product was colorless, gave 0.8 g. 5-(9-phenanthrylmethyl)-5-methylbarbituric acid, m. 233-5° (MePh). Refluxing 2.26 g. I in 62 ml. PrOH with 1.56 g. ethylbarbituric acid and 0.8 g. AcONa in 7 ml. H2O for 5 hrs., distilling the solvent, taking up with 100 ml. H2O, allowing to stand, and washing with C6H6 gave 1.2 g. 5-(9-phenanthrylmethyl)-5-ethylbarbituric acid (II), m. 237-8° (xylene). By an analogous procedure there were prepared the following analogs of II: 5-Pr, m. 240° (MePh); 5-Bu, m. 245-8° (MePh and C6H6); 5-allyl, m. 228-30° (xylene). Adding to 6.3 g. K2Cr2O7 in 19 g. H2SO4 and 31 ml. H2O at water bath temperature 2 1 g. I, adding later 6.3 g. K2Cr2O7, heating to boiling, cooling, diluting with H2O, washing thoroughly, digesting the solid with NaHSO3 solution at 50-60°, precipitating the phenanthrenequinone with dilute H2SO4 and subliming gave the pure quinone, m. 204°. Treating this quinone in EtOH with o-phenylenediamine gave the corresponding phenazine, m. 217°. Refluxing 2 g. II 48 hrs. with 20 ml. 25% NaOH solution and 20 ml. EtOH, diluting with H2O, acidifying with 10% H2SO4, keeping for crystallization, filtering, dissolving with NaHCO3 solution, precipitating with H2SO4, dissolving in Et2O, and precipitating with petr. ether gave 0.5 g. ethyl-(9-phenanthrylmethyl)malonic acid, m. 152-4° (decomposition). Refluxing 2.26 g. I with 1.58 g. 5-methyl-2-thiobarbituric acid in 60 ml. PrOH to dissoln., adding 0.8 g. NaOAc in 7 ml. H2O, refluxing 1 hr., distilling the PrOH to a small volume, adding 100 ml. H2O, washing the crystals with C6H6, dissolving repeatedly in NaOH and precipitating with HCl gave 2.15 g. 5-(9-phenanthrylmethyl)-5-methyl-2-thiobarbituric acid, m. 280-2°. By an analogous procedure with 0.1 mole material were prepared 3.4 g. 5-Et analog., 250-3° (xylene), 2.5 g. Pr analog. m. 230-1° (xylene), 0.8 g. Bu analog, m. 210° (xylene), and 0.8 g. allyl analog m. 185-9°(MePh). Dissolving 7.4 g. Na in 135 anhydrous EtOH, adding 8.5 g. thiourea and 20 g. di-Et allylmalonate, refluxing 4 hrs., dissolving the precipitate in a min. volume of H2O, and precipitating with HCl gave 3.52 g. 5-allyl-2-thiobarbituric acid, m. 120-2° (xylene). By the same method was prepared from 11.5 g. thiourea and 25 g. di-Et propylmalonate 5.37 g. 5-propyl-2-thiobarbituric acid, m. 163-5° (H2O).

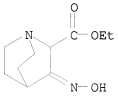
IT 34286-16-3 110056-51-4 117342-57-1
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 34286-16-3 CAPLUS

CN 1-Azabicyclo[2.2.2]octane-2-carboxylic acid, 3-oxo-, ethyl ester (CA INDEX NAME)

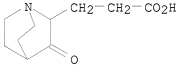


RN 110056-51-4 CAPLUS
CN 2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester, oxime, hydrochloride (6CI) (CA INDEX NAME)



● HCl

RN 117342-57-1 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



L15 ANSWER 132 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1959:122172 CAPLUS
DOCUMENT NUMBER: 53:122172
ORIGINAL REFERENCE NO.: 53:21953f-i,21954a-c
TITLE: Cyanoethylation of 3-quinuclidinone
AUTHOR(S): Mikhlina, E. E.; Rubtsov, M. V.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Sci. Research Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 118-24
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

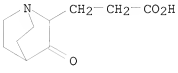
AB Na (24 g.) in 100 ml. MePh and 36 ml. absolute EtOH heated to 120-5°, treated over 1 hr. with 60 g. 1-carbethoxymethyl-4-carbethoxypiperidine in 150 ml. MePh, refluxed 5 hrs., treated with 200 ml. concentrated HCl, the mixture stirred 0.5 hr., the organic layer separated, reextd. with 200 ml. concentrated HCl twice, the acid exts. combined, refluxed 15 hrs., decolorized, and the residue evaporated, treated with 50% KOH, and extracted with C6H6 gave 84.6% 3-quinuclidinone, m. 136-8°; picrate, m. 210°. This (25 g.) in 115 ml. dry dioxane and 3.8 ml. 30% KOH in MeOH heated to 60°, treated over 0.5 hr. with 90 ml. CH2:CHCN, stirred 4 hrs. at 60°, the amorphous polymer filtered off, the filtrate freed of dioxane in vacuo, the residue treated with 100 ml. C6H6, extracted with 50 ml. 10% HCl, and the acid extract treated with K2CO3, and extracted with C6H6 yielded on distillation 14.3 g. 3-quinuclidinone. The distillation residue with 20 ml. absolute EtOH and 1 ml. dry C6H6 yielded 4 g. 3-oxo-2,2-bis(2-cyanoethyl)quinuclidine (Ia), m. 120-2° (EtOH); the mother liquor gave 0.7 g. 3-oxo-2-(2-cyanoethyl)quinuclidine (I), b0.3 121-2°. The same products were formed in Me3COH with MeOH-KOH catalyst. Refluxing I with HCl-AcOH 20 hrs. gave crude 3-oxo-2-(2-carboxyethyl)quinuclidine HCl salt, which, heated 3 hrs. with 9% alc.-dry HCl gave 60.6% 3-oxo-2-(2-carbethoxyethyl)quinuclidine (II), b0.4 136-8°, after the usual treatment of the mixture with K2CO3; the ester refluxed 4 hrs. with 17% HCl gave 96.5% 3-oxo-2-(2-carboxyethyl)quinuclidine HCl salt, decompose 191-3° (EtOH). Heating 0.3 g. II and 1.8 ml. N2H4.H2O with 0.4 g. Na in 9 ml. absolute EtOH in a sealed tube 14 hrs. at 170-80°, distilling the EtOH, refluxing the residue 4 hrs. with 10 ml. H2O, acidifying with HCl, evaporating, heating the residue with 10 ml. 10% alc. HCl 3 hrs., distilling the EtOH, treating the residue with K2CO3, and extracting with Et2O gave 0.17 g. 2-(2-carbethoxyethyl)quinuclidine, b0.2 90-2°, which, refluxed 4 hrs. with 17% HCl, gave 0.06 g. 2-(2-carboxyethyl)quinuclidine HCl salt, decompose 216.5-17.5°. Reduction of II with LiAlH4 in Et2O gave 56.7% 3-hydroxy-2-(3-hydroxypropyl)quinuclidine, b0.4 163-5°; HCl salt, m. 132-3°. Refluxing Ia with AcOH-concentrated HCl 17 hrs. gave 92% 3-oxo-2,2-bis(2-carboxyethyl)quinuclidine HCl salt, decompose 245° (90% EtOH). This refluxed 4 hrs. with 9% alc. HCl gave 63.6% 3-oxo-2,2-bis(2-carbethoxyethyl)quinuclidine (III), b1 190°, m. 58-61°; HCl salt, m. 169-71° (EtOH). Reductions of III with LiAlH4 in Et2O gave 85% 3-hydroxy-2,2-bis(3-hydroxypropyl)quinuclidine, hygroscopic crystals; HCl salt, m. 221-3° (EtOH). Keeping 0.35 g. III with 0.6 ml. N2H4.H2O in 2 ml. absolute EtOH 8 days gave 0.2 g. III dihydrazide, hygroscopic solid yielding a picrate, decompose 168°. Heating III with N2H4.H2O in EtOH-EtONa, as above, 14 hrs. at 160-70° gave 50% 2,2-bis(2-carbethoxyethyl)quinuclidine, b0.2 175-80°, which, refluxed 4 hrs. with 17% HCl, gave 30% 2,2-bis(2-carboxyethyl)quinuclidine HCl salt, decompose 215-18° (Me2CO-EtOH). Heating 1.2 g. LiAlH4, 1 g. Ia, 45 ml. C6H6, and 20 ml. absolute Et2O 40 hrs. at 65-70°, adding 3 ml. H2O, separating the inorg.

salts, washing these with dry pyridine, and evaporating the filtrate gave 59.6% 3-hydroxy-2,2-bis-(2-cyanoethyl)quinuclidine, m. 179-80° (absolute EtOH).

IT 75208-48-9 105339-98-8 105339-99-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 75208-48-9 CAPLUS

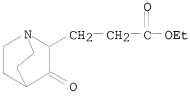
CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, 3-oxo-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 105339-98-8 CAPLUS

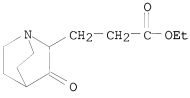
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester, hydrochloride (6CI) (CA INDEX NAME)



● HCl

RN 105339-99-9 CAPLUS

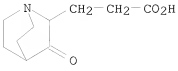
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester (6CI) (CA INDEX NAME)



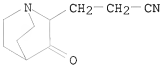
IT 117342-57-1, 2-Quinuclidinepropionic acid, 3-oxo-
(derivs.)

RN 117342-57-1 CAPLUS

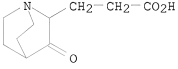
CN 2-Quinuclidinepropionic acid, 3-oxo- (6CI) (CA INDEX NAME)



IT 99169-54-7P, 2-Quinuclidinepropionitrile, 3-oxo-
RL: PREP (Preparation)
(preparation of)
RN 99169-54-7 CAPLUS
CN 2-Quinuclidinepropionitrile, 3-oxo- (6CI) (CA INDEX NAME)

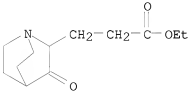


L15 ANSWER 133 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1959:122171 CAPLUS
DOCUMENT NUMBER: 53:122171
ORIGINAL REFERENCE NO.: 53:21953e-f
TITLE: Syntheses in the allo-lupinane series. IV. An alternative synthesis of 4-hydroxymethylquinolizidine
AUTHOR(S): Lukes, R.; Vesely, Z.
CORPORATE SOURCE: Vysoka skola chem. technol., Prague
SOURCE: Collection of Czechoslovak Chemical Communications (1959), 24, 2318-23
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: German
AB See C.A. 53, 368f.
IT 75208-48-9 105339-98-8 105339-99-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 75208-48-9 CAPLUS
CN 1-Azabicyclo[2.2.2]octane-2-propanoic acid, 3-oxo-, hydrochloride (9CI) (CA INDEX NAME)



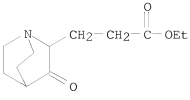
● HCl

RN 105339-98-8 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester, hydrochloride (6CI) (CA INDEX NAME)

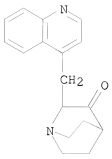


● HCl

RN 105339-99-9 CAPLUS
CN 2-Quinuclidinepropionic acid, 3-oxo-, ethyl ester (6CI) (CA INDEX NAME)



L15 ANSWER 134 OF 134 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1940:708 CAPLUS
DOCUMENT NUMBER: 34:708
ORIGINAL REFERENCE NO.: 34:110b-g
TITLE: Synthesis of 5-substituted rubans
AUTHOR(S): Clemo, G. R.; Hoggarth, E.
SOURCE: Journal of the Chemical Society (1939) 1241-4
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 34:708
GI For diagram(s), see printed CA Issue.
AB Lepidine (40 g.), 44 g. chloral and 100 cc. C5H5N, warmed at 85-90° for 2 hrs., give 80% of γ-trichloro-β-hydroxy-α-(4-quinolyl)propane, m. 178°; adding 65 g. during 2 hrs. to 65 g. KOH in 300 cc. absolute EtOH on the water bath gives 80% of β-4-quinolylacrylic acid, m. 270°; oxidation of 36 g. acid in a solution of 14 g. Na2CO3 in 500 cc. H2O with 60 g. KMnO4 in 1.5 l. H2O at -10° gives 58% (overall yield 38-40%) of quinoline-4-aldehyde (I), b4 122-3°, m. 52°; picrate, yellow, m. 179° (contains 1 mole of EtOH). 3-Ketoquinuclidine (II) (C. and Metcalfe, C. A. 32, 1701.3, term it the 2-derivative) and BzH in absolute EtOH containing piperidine or KOH, refluxed 8-10 hrs., give 2-benzylidene-3-ketoquinuclidine, light yellow, m. 133°; phenylhydrazone, light yellow, m. 184°. II (0.5 g.) and 0.8 g. I in AcOH, saturated with dry HCl at 0°, and after 2-3 hrs. warmed at 80-5° for 8 hrs., give 0.2 g. 5-keto-6,9-rubanene (III), deep yellow, m. 153°; III results in 0.4-0.5 g. yield from 0.5 g. II and 0.65 g. I with piperidine acetate in absolute EtOH; after keeping 60 hrs. in the cold and then heating momentarily to boiling; picrate, red, m. 209°; chloroplatinate, orange needles, decompose above 260° without melting. Catalytic reduction of 0.5 g. of III with Pd-C in MeOH gives 0.3 g. of 5-ketoruban (IV (R = 4-quinolyl)), m. 125-6°; phenylhydrazone, yellow, m. 198°; picrate, deep yellow, m. 168°. Reduction of 0.5 g. of IV with (iso-PrO)3Al in iso-PrOH gives 0.3 g. of ruban-5-ol, m. 198°; picrate, yellow, m. 188-9°. IV (0.3 g.) with EtMgI in Et2O at -10° gives 0.03-0.05 g. of 5-ethylruban-5-ol (V), m. 139°; picrate, yellow, m. 161°. III (0.8 g.) and EtMgI in Et2O at 0° give 0.05 g. of a compound C19H22ON2, m. 164°; picrate, deep yellow, m. 150°; crystalline compds. could not be prepared with N2H4.H2O, PhNHNH2, NH2OH or H2NNHCONH2; no Me2CO was detected in an attempted reduction with (iso-PrO)3Al and the compound was unchanged on boiling with HCO2H or Ac2O; catalytic reduction did not yield V.
IT 24177-70-6, 3-Quinuclidinone, 2-(4-quinolylmethyl)- (and derivs.)
RN 24177-70-6 CAPLUS
CN 11-Norcinchonan-7-one, (8ξ)- (9CI) (CA INDEX NAME)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